

=> b reg

FILE "REGISTRY" ENTERED AT 08:52:11 ON 03 JAN 2005

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STRUCTURE FILE UPDATES: 2 JAN 2005 HIGHEST RN 807298-39-1

DICTIONARY FILE UPDATES: 2 JAN 2005 HIGHEST RN 807298-39-1

TSCA INFORMATION NOW CURRENT THROUGH MAY 21, 2004

Please note that search-term pricing does apply when
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Crossover limits have been increased. See HELP CROSSOVER for details.

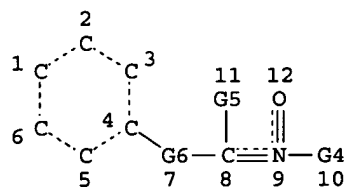
Experimental and calculated property data are now available. For more
information enter HELP PROP at an arrow prompt in the file or refer
to the file summary sheet on the web at:
<http://www.cas.org/ONLINE/DBSS/registryss.html>

=> d que stat 116

L3 SCR 2039 OR 2050 OR 2049 OR 2049 OR 2053 OR 2052 OR 2043

L4 SCR 1678 OR 1679 OR 1667

L6 STR



VAR G4=AK/CY

VAR G5=H/AK/CB

REP G6=(1-6) C

NODE ATTRIBUTES:

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

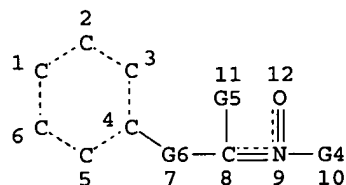
RSPEC 1

NUMBER OF NODES IS 12

STEREO ATTRIBUTES: NONE

L8 431 SEA FILE=REGISTRY SSS FUL L6 AND L4 NOT L3

L9 STR



VAR G4=AK/CY

VAR G5=H/AK/CB

REP G6=(1-6) CH2

NODE ATTRIBUTES:

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

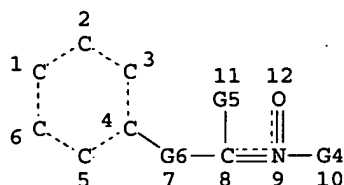
RSPEC 1
NUMBER OF NODES IS 12

STEREO ATTRIBUTES: NONE

L11 63 SEA FILE=REGISTRY SUB=L8 SSS FUL L9
L15 61 SEA FILE=REGISTRY ABB=ON PLU=ON L11 NOT C38H39N3O7
~~L16 48 SEA FILE=REGISTRY ABB=ON PLU=ON L15 NOT (C18H19NO OR
C11H16N2O OR C15H15NO OR C12H17NO OR C14H13NO OR C9H11NO OR
C38H39N3O7 OR C10H13NO)~~

=> d que stat L18

~~L3~~ SCR 2039 OR 2050 OR 2049 OR 2049 OR 2053 OR 2052 OR 2043
L4 SCR 1678 OR 1679 OR 1667
L6 STR



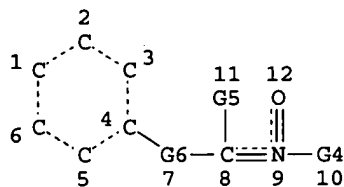
VAR G4=AK/CY
VAR G5=H/AK/CB
REP G6=(1-6) C
NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RSPEC 1
NUMBER OF NODES IS 12

STEREO ATTRIBUTES: NONE

L8 431 SEA FILE=REGISTRY SSS FUL L6 AND L4 NOT L3
L12 STR



C@13

VAR G4=AK/CY
VAR G5=H/AK/CB
REP G6=(1-6) 13
NODE ATTRIBUTES:
CONNECT IS M3 RC AT 13
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RSPEC 1
NUMBER OF NODES IS 13

STEREO ATTRIBUTES: NONE

L14 188 SEA FILE=REGISTRY SUB=L8 SSS FUL L12
~~L17 48 SEA FILE=REGISTRY ABB=ON PLU=ON L14 AND (C17H25NO OR
C10H13NO OR C18H14N2O5 OR C13H19NO OR C15H21NO OR C13H17NO OR
C22H31NO2SI OR C17H25NO3)~~

~~L18 3 SEA FILE=REGISTRY ABB=ON PLU=ON L17 AND (C10H13NO OR C13H19NO OR C17H25NO3)~~

=> d his

(FILE 'HOME' ENTERED AT 07:09:26 ON 03 JAN 2005)

FILE 'REGISTRY' ENTERED AT 07:12:10 ON 03 JAN 2005

L1 STR
L2 0 L1
L3 SCR 2039 OR 2050 OR 2049 OR 2049 OR 2053 OR 2052 OR 2043
L4 SCR 1678 OR 1679 OR 1667
L5 1 L1 AND L4 NOT L3
L6 STR L1
L7 2 L6 AND L4 NOT L3
L8 431 L6 AND L4 NOT L3 FULL
SAV TEM NWA0810F0/A L8
L9 STR L6
L10 4 L9 SAM SUB=L8
L11 63 L9 FULL SUB=L8
SAV TEM NWA0810S0/A L11
L12 STR L6
L13 10 L12 SAM SUB=L8
L14 188 L12 FULL SUB=L8
SAV TEM NWA0810S1/A L14
L15 61 L11 NOT C38H39N3O7
~~L16 48 L15 NOT (C18H19NO OR C11H16N2O OR C15H15NO OR C12H17NO OR C14H1~~

~~FILE 'REGISTRY' ENTERED AT 08:44:32 ON 03 JAN 2005~~

~~L17 8 L14 AND (C17H25NO OR C10H13NO OR C18H14N2O5 OR C13H19NO OR C15H~~
~~L18 3 L17 AND (C10H13NO OR C13H19NO OR C17H25NO3))~~

FILE 'HCAPLUS' ENTERED AT 08:47:12 ON 03 JAN 2005

L19 172 L11 OR L14
E KHAN M/AU
L20 893 E3-5,E57
E UPASANI R/AU
L21 62 E3-10
E WOOD P/AU
L22 639 E3-30
E WOOD PAUL/AU
L23 168 E3,E11
E WOOD PAUL L/AU
L24 1 L19 AND L20-23
L25 17 L16 OR L18
L26 1 L25 AND L20-23
~~L27 1 L24 OR L26~~
~~L28 16 L25 NOT L27~~

FILE 'HCAOLD' ENTERED AT 08:51:45 ON 03 JAN 2005

L29 0 L16 OR L18

=> b hcap

FILE 'HCAPLUS' ENTERED AT 08:52:28 ON 03 JAN 2005

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FILE COVERS 1907 - 3 Jan 2005 VOL 142 ISS 2
FILE LAST UPDATED: 31 Dec 2004 (20041231/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

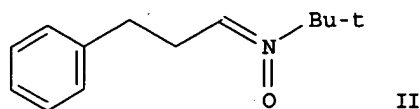
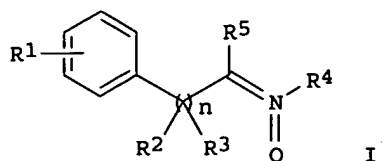
~~and al. Chitester, 127~~

L27 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2005 ACS on STN
AN 2004:354748 HCAPLUS
DN 140:374898
ED Entered STN: 30 Apr 2004
TI Preparation of nitron compounds and methods for treating inflammation and neuropathic pain
IN Khan, M. Amin; Upasani, Ravindra B.; Wood, Paul
L.
PA Renovis, Inc., USA
SO PCT Int. Appl., 56 pp.
CODEN: PIXXD2
DT Patent
LA English
IC ICM A61K
CC 23-4 (Aliphatic Compounds)
Section cross-reference(s): 1, 63
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2004034999	A2	20040429	WO 2003-US32883	20031015
	WO 2004034999	A3	20040617		
	W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW			
	RW:	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
	US 2004142983	A1	20040722	US 2003-684810	20031014
PRAI	US 2002-419029P	P	20021015		
	US 2003-684810	A	20031014		

CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
WO 2004034999	ICM	A61K
OS	MARPAT 140:374898	
GI		



- AB Title compds. I [n = 1-6; R1 = H, alk(en/yn)yl, cycloalkyl, etc.; R2-3, R5 = H, (cyclo)alkyl; R4 = alkyl, cycloalkyl, cycloalkylalkylene, aryl, aralkyl] are prepared For instance, 3-phenylpropionaldehyde is reacted with N-(tert-butyl)hydroxylamine (PhH/CHCl3, reflux (with water removal), 22 h) to give II. I are useful as therapeutics for inflammation-related conditions and analgesia in mammals, such as arthritis, and for neuropathic pain and traumatic injuries such as traumatic brain injury and acute spinal cord injury. The invention accordingly extends to the use of the compds. and compns. for the stated treatments, and as appropriate, to the use of the compds. for the preparation of pharmaceutical compns. for such treatments.
- ST nitron inflammation neuropathic pain prepn
- IT Spinal cord, disease
(injury; preparation of nitron compds. and methods for treating inflammation and neuropathic pain)
- IT Analgesics
Anti-inflammatory agents
Human
Inflammation
Pain
(preparation of nitron compds. and methods for treating inflammation and neuropathic pain)
- IT Brain, disease
(trauma; preparation of nitron compds. and methods for treating inflammation and neuropathic pain)
- IT 82937-45-9P 85664-58-0P, N-tert-Butyl[[1-(phenyl)ethyl]methylene]amine N-oxide 367523-81-7P, N-tert-Butyl[[2-(phenylethyl)methylene]amine N-oxide 683746-73-8P, N-tert-Butyl[[2-[4-(methoxymethoxy)phenyl]ethyl]methylene]amine N-oxide 683746-74-9P, N-tert-Butyl[[2-(4-hydroxyphenyl)ethyl]methylene]amine N-oxide 683746-75-0P, N-tert-Butyl[[2-(4-methoxyphenyl)ethyl]methylene]amine N-oxide 683746-76-1P, N-tert-Butyl[[2-[4-(tetrahydropyran-2-yloxy)phenyl]ethyl]methylene]amine N-oxide 683746-77-2P, N-tert-Butyl[[2-(4-isopropoxyphenyl)ethyl]methylene]amine N-oxide 683746-79-4P, N-tert-Butyl[[2-(4-ethoxyphenyl)ethyl]methylene]amine N-oxide 683746-80-7P, N-tert-Butyl[[2-[4-(benzenesulfonyloxy)phenyl]ethyl]methylene]amine N-oxide 683746-83-0P, N-tert-Butyl[[2-[4-(acetamido)phenyl]ethyl]methylene]amine N-oxide 683746-84-1P, N-tert-Butyl[[2-[4-((benzenesulfonyl)amino)carbonyl]phenyl]ethyl]methylene]amine N-oxide 683746-86-3P 683746-89-6P, N-tert-Butyl[(5-phenylpentyl)methylene]amine N-oxide 683746-90-9P, N-tert-Butyl[[2-(4-isopropylphenyl)-1-methylethyl]methylene]amine N-oxide 683746-91-0P, N-tert-Butyl[(3-phenylpropyl)methylene]amine N-oxide 683746-92-1P, N-tert-Butyl[[1-(4-tert-butylbenzyl)ethyl]methylene]amine N-oxide 683746-93-2P, N-tert-Butyl[[2-(4-methoxyphenyl)-1-

methylethyl)methylene]amine N-oxide 683746-94-3P,
 N-Cyclohexyl[(2-phenylethyl)methylene]amine N-oxide 683746-95-4P
 , N-tert-Butyl[(4-phenylbutyl)methylene]amine N-oxide 683746-96-5P
 , N-tert-Butyl[(2-{3,5-di-(tert-butyl)-4-hydroxyphenyl}ethyl)methylene]ami
 ne N-oxide 683746-97-6P 683746-98-7P,
 N-tert-Butyl[[3-(4-methoxyphenyl)propyl)methylene]amine N-oxide
 683746-99-8P 683747-00-4P 683747-01-5P
 683747-02-6P 683747-03-7P 683747-04-8P
 683747-05-9P 683747-06-0P 683747-07-1P
 683747-08-2P 683747-09-3P 683747-10-6P
 683747-11-7P 683747-12-8P 683747-13-9P
 RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
 (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
 (Uses)

(preparation of nitron compds. and methods for treating inflammation and
 neuropathic pain)

IT 75-03-6, Iodoethane 75-30-9, 2-Iodopropane 80-54-6,
 2-[(4-tert-Butylphenyl)methyl]propanal 93-53-8, 2-Phenylpropanal
 98-09-9, Benzenesulfonyl chloride 103-95-7, 2-Methyl-3-(4-
 isopropylphenyl)propionaldehyde 104-53-0, 3-Phenylpropionaldehyde
 107-18-6, Allyl alcohol, reactions 107-30-2, Chloromethyl methyl ether
 110-87-2, 3,4-Dihydro-2H-pyran 122-78-1, Phenylacetaldehyde 501-97-3,
 3-(4-Hydroxyphenyl)propionic acid 540-37-4, 4-Iodoaniline 2211-64-5,
 N-Cyclohexylhydroxylamine 2430-16-2, 6-Phenylhexanol 16649-50-6,
 N-tert-Butylhydroxylamine 18328-11-5, 4-Phenylbutyraldehyde
 20401-88-1, 3-(4-Methoxyphenyl)propanal 33551-58-5, 2-(3,5-Di-tert-butyl-
 4-hydroxyphenyl)ethanal 36884-28-3, 5-Phenylpentanal 54685-32-4,
 3-(3,5-Di-tert-butyl-4-hydroxyphenyl)propanal 56047-51-9,
 4-(4-Methoxyphenyl)butanal

RL: RCT (Reactant); RACT (Reactant or reagent)

(preparation of nitron compds. and methods for treating inflammation and
 neuropathic pain)

IT 622-50-4P, N-(4-Iodophenyl)acetamide 10210-17-0P, 3-(4-Hydroxyphenyl)-1-
 propanol 16387-61-4P, 6-Phenylhexanal 20238-83-9P,
 3-(4-Hydroxyphenyl)propanal 63537-11-1P, 3-(4-Ethoxyphenyl)propanal
 72457-43-3P, 3-(4-Ethoxyphenyl)-1-propanol 74882-15-8P,
 3-[4-(Methoxymethoxy)phenyl]-1-propanol 74882-16-9P,
 3-[4-(Methoxymethoxy)phenyl]propanal 154498-20-1P, 4-
 ((Benzenesulfonyl)amino)carbonyl)-1-iodobenzene 169054-06-2P,
 3-[4-(Acetamido)phenyl]propanal 256946-22-2P, 3-[4-(Tetrahydropyran-2-
 yloxy)phenyl]propanal 365572-36-7P, 3-[4-(Isopropoxy)phenyl]-1-propanol
 683746-78-3P, 3-[4-(Isopropoxy)phenyl]propanal 683746-81-8P
 683746-82-9P, 3-[4-(Benzenesulfonyloxy)phenyl]propanal 683746-85-2P,
 3-[4-(((Benzenesulfonyl)amino)carbonyl)phenyl]propanal 683746-87-4P
 683746-88-5P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)

(preparation of nitron compds. and methods for treating inflammation and
 neuropathic pain)

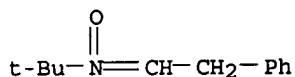
IT 82937-45-9P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
 (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
 (Uses)

(preparation of nitron compds. and methods for treating inflammation and
 neuropathic pain)

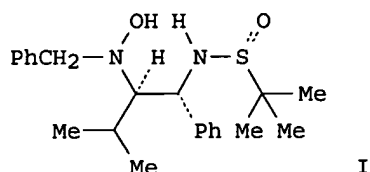
RN 82937-45-9 HCAPLUS

CN 2-Propanamine, 2-methyl-N-(2-phenylethylidene)-, N-oxide (9CI) (CA INDEX
 NAME)



→ d all hitstr 128 tot

L28 ANSWER 1 OF 16 HCAPLUS COPYRIGHT 2005 ACS on STN
 AN 2004:800218 HCAPLUS
 DN 141:423969
 ED Entered STN: 01 Oct 2004
 TI Samarium diiodide-induced asymmetric synthesis of optically pure unsymmetrical vicinal diamines by reductive cross-coupling of nitrones with N-tert-butanefulfinyl imines
 AU Zhong, Yu-Wu; Xu, Ming-Hua; Lin, Guo-Qiang
 CS Shanghai Institute of Organic Chemistry, Chinese Academy of Sciences, Shanghai, 200032, Peop. Rep. China
 SO Organic Letters (2004), 6(22), 3953-3956
 CODEN: ORLEF7; ISSN: 1523-7060
 PB American Chemical Society
 DT Journal
 LA English
 CC 23-4 (Aliphatic Compounds)
 Section cross-reference(s): 75
 GI



AB An efficient method for the preparation of optically pure unsym. vicinal diamines, e.g., I, by the SmI2-induced reductive cross-coupling of nitrones with chiral N-tert-butanefulfinyl imines was developed. This is a successful example of the highly diastereoselective and enantioselective cross-coupling between two different imine species. It provides a straightforward access to enantiopure unsym. vicinal diamines that are widely applicable in asym. synthesis.

ST nitrone chiral sulfinyl imine reductive cross coupling samarium; diamine asym prepn; samarium asym reductive cross coupling mediator

IT Imines
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (chiral, sulfinyl; stereoselective preparation of N-benzyl-N-hydroxy-N'-(t-butylsulfinyl)alkanediamines via samarium-mediated asym. reductive cross-coupling of chiral N-t-butylsulfinyl imines with nitrones)

IT Amines, preparation
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (diamines; stereoselective preparation of N-benzyl-N-hydroxy-N'-(t-butylsulfinyl)alkanediamines via samarium-mediated asym. reductive cross-coupling of chiral N-t-butylsulfinyl imines with nitrones)

IT Crystal structure
 Molecular structure
 (of N-benzyl-N-hydroxy-N'-(t-butylsulfinyl)methyl(phenyl)butanediamine)

IT Asymmetric synthesis and induction
 (stereoselective preparation of N-benzyl-N-hydroxy-N'-(t-butylsulfinyl)alkanediamines via samarium-mediated asym. reductive cross-coupling of chiral N-t-butylsulfinyl imines with nitrones)

IT Nitrones
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (stereoselective preparation of N-benzyl-N-hydroxy-N'-(t-butylsulfinyl)alkanediamines via samarium-mediated asym. reductive cross-coupling of chiral N-t-butylsulfinyl imines with nitrones)

- IT Cross-coupling reaction
(stereoselective, reductive; stereoselective preparation of N-benzyl-N-hydroxy-N'-(t-butylsulfinyl)alkanediamines via samarium-mediated asym. reductive cross-coupling of chiral N-t-butylsulfinyl imines with nitrones)
- IT 195059-76-8
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of N,N'-diacetyl(methyl)phenylbutanediamines via acetylation of methyl(phenyl)butanediamines)
- IT 796038-90-9P 796038-91-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of N,N'-diacetyl(methyl)phenylbutanediamines via acetylation of methyl(phenyl)butanediamines)
- IT 796038-88-5P 796038-89-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of methyl(phenyl)butanediamine hydrochloride via deoxygenation of N-benzyl-N-hydroxy-N'-(t-butylsulfinyl)methyl(phenyl)butanediamine followed by hydrolysis and hydrogenation)
- IT 796038-69-2P
RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(stereoselective preparation and crystal structure of N-benzyl-N-hydroxy-N'-(t-butylsulfinyl)methyl(phenyl)butanediamine via samarium-mediated asym. reductive cross-coupling of N-t-butylsulfinyl benzaldehyde imine with benzyl(t-butyl)nitron)
- IT 115869-93-7 186249-76-3
RL: RCT (Reactant); RACT (Reactant or reagent)
(stereoselective preparation and crystal structure of N-benzyl-N-hydroxy-N'-(t-butylsulfinyl)methyl(phenyl)butanediamine via samarium-mediated asym. reductive cross-coupling of N-t-butylsulfinyl benzaldehyde imine with benzyl(t-butyl)nitron)
- IT 22687-06-5 105798-17-2 144433-08-9 162365-56-2 244092-54-4
336105-23-8 336105-24-9 439129-59-6 796038-70-5
796038-71-6 796038-72-7 796038-73-8 796038-74-9
RL: RCT (Reactant); RACT (Reactant or reagent)
(stereoselective preparation of N-benzyl-N-hydroxy-N'-(t-butylsulfinyl)alkanediamines via samarium-mediated asym. reductive cross-coupling of chiral N-t-butylsulfinyl imines with nitrones)
- IT 32248-43-4, Samarium diiodide
RL: RGT (Reagent); RACT (Reactant or reagent)
(stereoselective preparation of N-benzyl-N-hydroxy-N'-(t-butylsulfinyl)alkanediamines via samarium-mediated asym. reductive cross-coupling of chiral N-t-butylsulfinyl imines with nitrones)
- IT 796038-75-0P 796038-76-1P 796038-77-2P 796038-78-3P 796038-79-4P
796038-80-7P 796038-81-8P 796038-82-9P 796038-83-0P 796038-84-1P
796038-85-2P 796038-86-3P 796038-87-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(stereoselective preparation of N-benzyl-N-hydroxy-N'-(t-butylsulfinyl)alkanediamines via samarium-mediated asym. reductive cross-coupling of chiral N-t-butylsulfinyl imines with nitrones)
- RE.CNT 43 THERE ARE 43 CITED REFERENCES AVAILABLE FOR THIS RECORD
- RE
- (1) Alexakis, A; Angew Chem, Int Ed 2000, V39, P4093 HCAPLUS
 - (2) Annunziata, R; Tetrahedron:Asymmetry 2002, V13, P2727 HCAPLUS
 - (3) Cogan, D; J Am Chem Soc 1998, V120, P8011 HCAPLUS
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 - (5) Dhavale, D; Liebigs Ann Chem 1992, P1289 HCAPLUS
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 - (8) Ellman, J; J Org Chem 2003, V68, P9948
 - (9) Itsuno, S; Tetrahedron Lett 2003, V44, P3825 HCAPLUS
 - (10) Jacobsen, E; J Org Chem 1994, V59, P1939
 - (11) Kagan, H; Tetrahedron 2003, V59, P10351 HCAPLUS
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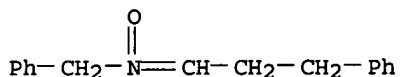
- (14) Krief, A; Chem Rev 1999, V99(9), P745
- (15) Liu, G; J Org Chem 1999, V64, P1278 HCAPLUS
- (16) Lucet, D; Angew Chem, Int Ed 1998, V37, P2580 HCAPLUS
- (17) Machrouhi, F; Tetrahedron Lett 1999, V40, P1315 HCAPLUS
- (18) Masson, G; Angew Chem, Int Ed 2002, V41, P1772 HCAPLUS
- (19) Masson, G; Angew Chem, Int Ed 2003, V42, P2265 HCAPLUS
- (20) Merino, P; Tetrahedron: Asymmetry 1997, V8, P2381 HCAPLUS
- (21) Molander, G; Chem Rev 1996, V96, P307 HCAPLUS
- (22) Molander, G; Tetrahedron 1998, V54, P3321 HCAPLUS
- (23) Muniz, K; Angew Chem, Int Ed 2003, V42, P5958 HCAPLUS
- (24) Muniz, K; Chem-Eur J 2003, V9, P5581 HCAPLUS
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IT 796038-70-5

RL: RCT (Reactant); RACT (Reactant or reagent)
 (stereoselective preparation of N-benzyl-N-hydroxy-N'-(t-butylsulfinyl)alkanediamines via samarium-mediated asym. reductive cross-coupling of chiral N-t-butylsulfinyl imines with nitrones)

RN 796038-70-5 HCAPLUS

CN Benzenemethanamine, N-(3-phenylpropylidene)-, N-oxide (9CI) (CA INDEX NAME)



L28 ANSWER 2 OF 16 HCAPLUS COPYRIGHT 2005 ACS on STN

AN 2004:715426 HCAPLUS

DN 141:365963

ED Entered STN: 02 Sep 2004

TI Radical addition of nitrones to acrylates mediated by SmI2: asymmetric synthesis of .gamma.-amino acids employing carbohydrate-based chiral auxiliaries

AU Johannesen, Sine A.; Albu, Silvia; Hazell, Rita G.; Skrydstrup, Troels

CS Department of Chemistry, University of Aarhus, Aarhus, Den.

SO Chemical Communications (Cambridge, United Kingdom) (2004), (17), 1962-1963

CODEN: CHCOFS; ISSN: 1359-7345

PB Royal Society of Chemistry

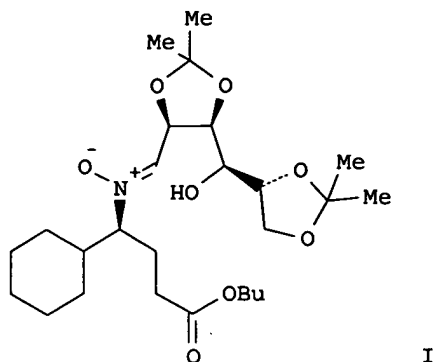
DT Journal

LA English

CC 23-17 (Aliphatic Compounds)

Section cross-reference(s): 33, 75

GI



- AB Alkyl nitrones possessing N-substituted sugars as chiral auxiliaries were found to effectively undergo an SmI2-mediated radical addition to Bu acrylate affording .gamma.-amino acid derivs., e.g. I, with high diastereomeric control.
- ST asym synthesis amino acid stereoselective radical addn nitron acrylate; carbohydrate chiral auxiliary stereoselective radical addn nitron acrylate; crystal mol structure amino acid carbohydrate chiral auxiliary
- IT Asymmetric synthesis and induction
Chiral auxiliary
(asym. synthesis of .gamma.-amino acids employing carbohydrate-based chiral auxiliaries via radical addition of nitrones to Bu acrylate mediated by SmI2)
- IT Nitrones
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(asym. synthesis of .gamma.-amino acids employing carbohydrate-based chiral auxiliaries via radical addition of nitrones to Bu acrylate mediated by SmI2)
- IT Addition reaction
(homolytic; asym. synthesis of .gamma.-amino acids employing carbohydrate-based chiral auxiliaries via radical addition of nitrones to Bu acrylate mediated by SmI2)
- IT Crystal structure
Molecular structure
(of .gamma.-amino acids produced employing carbohydrate-based chiral auxiliaries via radical addition of nitrones to Bu acrylate mediated by SmI2)
- IT Amino acids, preparation
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(.gamma.-amino acids; asym. synthesis of .gamma.-amino acids employing carbohydrate-based chiral auxiliaries via radical addition of nitrones to Bu acrylate mediated by SmI2)
- IT 780765-87-9P
RL: BPN (Biosynthetic preparation); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(asym. synthesis of .gamma.-amino acids employing carbohydrate-based chiral auxiliaries via radical addition of nitrones to Bu acrylate mediated by SmI2)
- IT 141-32-2 40036-82-6 101040-18-0 497155-65-4 780765-72-2
780765-76-6 780765-77-7 780765-78-8 780765-83-5 780765-84-6
780765-88-0
RL: RCT (Reactant); RACT (Reactant or reagent)
(asym. synthesis of .gamma.-amino acids employing carbohydrate-based chiral auxiliaries via radical addition of nitrones to Bu acrylate mediated by SmI2)
- IT 780765-74-4P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(asym. synthesis of .gamma.-amino acids employing carbohydrate-based chiral auxiliaries via radical addition of nitrones to Bu acrylate mediated by SmI2)

IT 780765-71-1P 780765-75-5P 780765-80-2P 780765-81-3P 780765-82-4P
780765-85-7P 780765-86-8P 780765-89-1P

RL: SPN (Synthetic preparation); PREP (Preparation)

(asym. synthesis of .gamma.-amino acids employing carbohydrate-based chiral auxiliaries via radical addition of nitrones to Bu acrylate mediated by SmI2)

IT 780765-73-3P 780765-79-9P

RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(crystal structure; asym. synthesis of .gamma.-amino acids employing carbohydrate-based chiral auxiliaries via radical addition of nitrones to Bu acrylate mediated by SmI2)

RE.CNT 10 THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS RECORD

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IT 780765-88-0

RL: RCT (Reactant); RACT (Reactant or reagent)

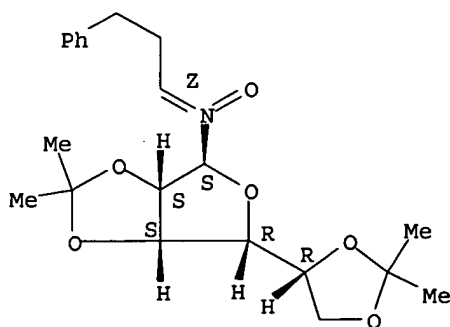
(asym. synthesis of .gamma.-amino acids employing carbohydrate-based chiral auxiliaries via radical addition of nitrones to Bu acrylate mediated by SmI2)

RN 780765-88-0 HCAPLUS

CN .alpha.-D-Mannofuranosylamine, 2,3:5,6-bis-O-(1-methylethylidene)-N-(3-phenylpropylidene)-, N-oxide, [N(Z)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.



L28 ANSWER 3 OF 16 HCAPLUS COPYRIGHT 2005 ACS on STN

AN 2004:394413 HCAPLUS

DN 141:106151

ED Entered STN: 16 May 2004

TI NMR Investigations of the .beta.-Cyclodextrin Inclusion of (.alpha.-Phenyl-N-tert-butyl-nitrone) Analogues

AU Bardelang, David; Clement, Jean-Louis; Finet, Jean-Pierre; Karoui, Hakim; Tordo, Paul

CS Laboratoire SREP UMR 6517, CNRS et Universites d'Aix-Marseille 1 et 3,

Marseille, 13397, Fr.

SO Journal of Physical Chemistry B (2004), 108(23), 8054-8061
CODEN: JPCBFK; ISSN: 1520-6106

PB American Chemical Society

DT Journal

LA English

CC 22-10 (Physical Organic Chemistry)
Section cross-reference(s): 77, 80

AB Recently, cyclodextrin derivs. were reported to increase significantly the half-life of the spin adducts resulting from the trapping of free radicals with nitrones. To address the physicochem. characteristics of these complexes, a series of .alpha.-phenyl-N-tert-butyl nitron (PBN) analogs containing hydroxy groups on the tert-Bu group was prepared. The influence of the substitution on the supramol. complexation of the nitrones with natural .beta.-cyclodextrin was studied by NMR spectroscopy. 1D-NMR studies indicated a 1:1 stoichiometry and binding consts. in the range 32 to 1075 M⁻¹ depending on the substitution pattern. 2D-NMR expts. suggested a competitive inclusion of the PBN derivs. by the aryl moiety through the two accessible wide and narrow rims of the cyclodextrin.

ST NMR cyclodextrin inclusion phenyl tertbutyl nitron analog

IT Stoichiometry
(1:1; association consts. and NMR on .beta.-cyclodextrin inclusion of (.alpha.-phenyl-N-tert-butyl nitron) analogs)

IT Titration
(NMR; association consts. and NMR on .beta.-cyclodextrin inclusion of (.alpha.-phenyl-N-tert-butyl nitron) analogs)

IT Formation constant
NMR (nuclear magnetic resonance)
Substituent effects
(association consts. and NMR on .beta.-cyclodextrin inclusion of (.alpha.-phenyl-N-tert-butyl nitron) analogs)

IT Inclusion compounds
RL: FMU (Formation, unclassified); FORM (Formation, nonpreparative)
(association consts. and NMR on .beta.-cyclodextrin inclusion of (.alpha.-phenyl-N-tert-butyl nitron) analogs)

IT Nitrones
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(association consts. and NMR on .beta.-cyclodextrin inclusion of (.alpha.-phenyl-N-tert-butyl nitron) analogs)

IT 719304-72-0 719304-74-2 719304-76-4 719304-78-6 719304-80-0
719304-82-2 719304-85-5 719304-87-7
RL: FMU (Formation, unclassified); FORM (Formation, nonpreparative)
(association consts. and NMR on .beta.-cyclodextrin inclusion of (.alpha.-phenyl-N-tert-butyl nitron) analogs)

IT 55277-95-7P 63829-51-6P 63829-61-8P 63829-70-9P 63829-90-3P
65102-43-4P 65102-45-6P 719304-01-5P 719304-06-0P 719304-12-8P
719304-17-3P 719304-84-4P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(association consts. and NMR on .beta.-cyclodextrin inclusion of (.alpha.-phenyl-N-tert-butyl nitron) analogs)

IT 76-39-1 77-49-6 100-52-7, Benzaldehyde, reactions 104-53-0,
Benzenepropanal 104-87-0 104-88-1, reactions 122-03-2 123-11-5,
reactions 555-16-8, reactions 939-97-9 3218-36-8,
[1,1'-Biphenyl]-4-carboxaldehyde 4748-78-1 21527-52-6
RL: RCT (Reactant); RACT (Reactant or reagent)
(association consts. and NMR on .beta.-cyclodextrin inclusion of (.alpha.-phenyl-N-tert-butyl nitron) analogs)

RE.CNT 36 THERE ARE 36 CITED REFERENCES AVAILABLE FOR THIS RECORD

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IT 719304-85-5

RL: FMU (Formation, unclassified); FORM (Formation, nonpreparative)
(association consts. and NMR on .beta.-cyclodextrin inclusion of
(.alpha.-phenyl-N-tert-butyl nitron) analogs)

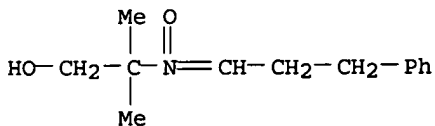
RN 719304-85-5 HCAPLUS

CN .beta.-Cyclodextrin, compd. with 2-methyl-2-[oxido(3-phenylpropylidene)amino]-1-propanol (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 719304-84-4

CMF C13 H19 N O2



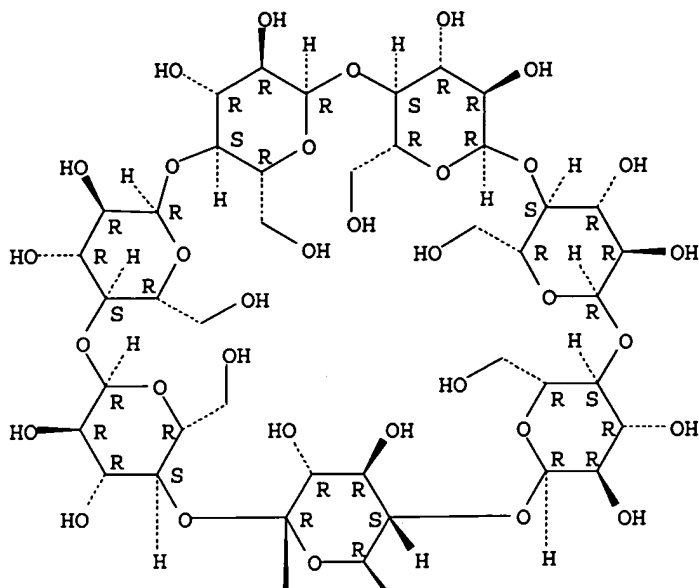
CM 2

CRN 7585-39-9

CMF C42 H70 O35

Absolute stereochemistry.

PAGE 1-A



PAGE 2-A

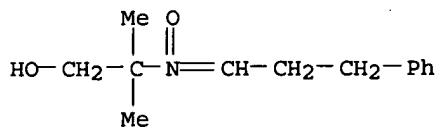


IT 719304-84-4P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
 (association consts. and NMR on .beta.-cyclodextrin inclusion of
 (.alpha.-phenyl-N-tert-butyl nitron) analogs)

RN 719304-84-4 HCAPLUS

CN 1-Propanol, 2-methyl-2-[oxido(3-phenylpropylidene)amino]- (9CI) (CA INDEX
 NAME)



L28 ANSWER 4 OF 16 HCAPLUS COPYRIGHT 2005 ACS on STN

AN 2003:786727 HCAPLUS

DN 139:365001

ED Entered STN: 08 Oct 2003

TI Dimethylzinc-promoted vinylation of nitrones with vinylboronic esters of
 pinacol: a new route to N-allylic hydroxylamines

AU Pandya, Shashi U.; Pinet, Sandra; Chavant, Pierre Y.; Vallee, Yannick

CS Department of Chemistry, Sardar Patel University, Gujarat, 388120, India

SO European Journal of Organic Chemistry (2003), (18), 3621-3627

CODEN: EJOCFK; ISSN: 1434-193X

PB Wiley-VCH Verlag GmbH & Co. KGaA

DT Journal

Search done by Noble Jarrell

- LA English
 CC 29-4 (Organometallic and Organometalloidal Compounds)
 Section cross-reference(s): 21
 OS CASREACT 139:365001
 AB Activation of pinacol vinylboronic esters with dimethylzinc allows nucleophilic addition of the vinyl group onto nitrones, producing N-allylic hydroxylamines in excellent yields. Reaction of 2-R1CH:CH-4,4,5,5-tetramethyl-1,3,2-dioxaborolanes (1a-f; R1 = Bu, C10H21, 1-cyclohexenyl, (CH2)3Cl, CH2CH2OPiv, CH2OtBu; prepared by reaction of CH.tplbond.CR1 with pinacolborane) with nitrones R2N+(O-):CHR3 in the presence of dimethyl- or diethylzinc gave hydroxylamines R2N(OH)CHR3CH:CHR1 (4a-1; R2 = PhCH2, Me, iPr, 1-naphthylmethyl; R3 = Ph, 4-CF3C6H4, 2-furyl, 1-phenylethyl, iBu). The presence of dialkylzinc in excess is essential for the reaction completion and yield of the hydroxylamines; the suggestions on the reaction mechanism are discussed.
- ST vinylboronate addn nitrone dialkylzinc promoted allylhydroxylamine prepn;
 alkyne pinacolborane vinylboronate nitrone addn allylhydroxylamine prepn
- IT Vinylation
 (addition of vinylboronates to nitrones promoted by dialkylzinc to give allylhydroxylamines)
- IT Nitrones
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (addition of vinylboronates to nitrones promoted by dialkylzinc to give allylhydroxylamines)
- IT Acids, preparation
 Group IIIA element compounds
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (boronic acids, esters, vinylboronates; preparation of vinylboronates by alkyne addition to pinacolborane and their dialkylzinc-promoted addition to nitrones to give allylhydroxylamines)
- IT Vinyl compounds, preparation
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (dialkylzinc-promoted addition of vinylboronates to nitrones to give allylhydroxylamines)
- IT Amines, preparation
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (hydroxylamines, vinyl-; preparation of allylhydroxylamines by dialkylzinc-promoted addition of vinylboronates to nitrones)
- IT Addition reaction
 (nucleophilic; dialkylzinc-promoted addition of vinylboronates to nitrones to give allylhydroxylamines)
- IT Alkynes
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (preparation of allylhydroxylamines by addition of alkynes to pinacolborane with subsequent dialkylzinc-promoted addition of vinylboronates to nitrones)
- IT 190072-42-5P, 2-Phenyl-4-nonen-3-ol 620635-12-3P, N-Benzyl-N-(4-tert-butoxy-1-phenyl-2-butenyl)hydroxylamine 620635-13-4P,
 1-Phenyl-1,4-pentadecadien-3-ol 620635-14-5P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of allyl alcs. by addition of alkynes to pinacolborane with subsequent dialkylzinc-promoted addition of vinylboronates to aldehydes and ketones)
- IT 390423-36-6P, N-Benzyl-N-(1-phenylpropyl)hydroxylamine 471256-90-3P,
 N-Benzyl-N-(1-phenylethyl)hydroxylamine 620635-05-4P
 RL: BYP (Byproduct); PREP (Preparation)
 (preparation of allylhydroxylamines by addition of alkynes to pinacolborane with subsequent dialkylzinc-promoted addition of vinylboronates to nitrones)
- IT 544-97-8, Dimethylzinc
 RL: MSC (Miscellaneous)
 (preparation of allylhydroxylamines by addition of alkynes to pinacolborane with subsequent dialkylzinc-promoted addition of vinylboronates to nitrones)

- IT 154820-94-7P 154820-95-8P, 2-(5-Chloro-1-pentenyl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane 620634-95-9P, 2-(1-Dodecenyl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane 620634-96-0P, 2-[2-(1-Cyclohexenyl)ethenyl]-4,4,5,5-tetramethyl-1,3,2-dioxaborolane 620634-97-1P, 4,4,5,5-Tetramethyl-2-(4-pivaloyloxy-1-butenyl)-1,3,2-dioxaborolane 620634-98-2P, 2-(3-tert-Butoxy-1-propenyl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (preparation of allylhydroxylamines by addition of alkynes to pinacolborane with subsequent dialkylzinc-promoted addition of vinylboronates to nitrones)
- IT 145526-91-6P 620634-99-3P, N-Benzyl-N-(1-phenyl-2-heptenyl)hydroxylamine 620635-00-9P, N-Benzyl-N-[1-(4-trifluoromethylphenyl)-2-heptenyl]hydroxylamine 620635-01-0P 620635-02-1P, O-[1-Butyl-3-(2-furanyl)-2-propenyl]-N-isopropylhydroxylamine 620635-04-3P 620635-06-5P, N-Benzyl-N-(1-phenyl-2-tridecenyl)hydroxylamine 620635-07-6P, N-Benzyl-N-(6-chloro-1-phenyl-2-hexenyl)hydroxylamine 620635-08-7P, N-Benzyl-N-[3-(1-cyclohexenyl)-1-phenyl-2-propenyl]hydroxylamine 620635-09-8P 620635-10-1P 620635-11-2P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of allylhydroxylamines by addition of alkynes to pinacolborane with subsequent dialkylzinc-promoted addition of vinylboronates to nitrones)
- IT 620635-03-2, N-[1-(2-Furanyl)-2-heptenyl]-N-isopropylhydroxylamine
 RL: FMU (Formation, unclassified); RCT (Reactant); FORM (Formation, nonpreparative); RACT (Reactant or reagent)
 (rearrangement, O-vinylation; preparation of allylhydroxylamines by addition of alkynes to pinacolborane with subsequent dialkylzinc-promoted addition of vinylboronates to nitrones)
- IT 93-53-8, 2-Phenylpropanal 104-55-2, Cinnamaldehyde 119-61-9, Benzophenone, reactions
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (vinylation; preparation of allyl alcs. by addition of alkynes to pinacolborane with subsequent dialkylzinc-promoted addition of vinylboronates to aldehydes and ketones)
- IT 3376-26-9 24423-87-8, 3,4-Dihydroisoquinoline-N-oxide 367523-77-1 426822-59-5 510773-86-1 620635-15-6 620635-16-7
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (vinylation; preparation of allylhydroxylamines by addition of alkynes to pinacolborane with subsequent dialkylzinc-promoted addition of vinylboronates to nitrones)

RE.CNT 38 THERE ARE 38 CITED REFERENCES AVAILABLE FOR THIS RECORD

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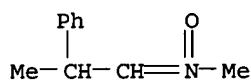
IT 426822-59-5

RL: RCT (Reactant); RACT (Reactant or reagent)

(vinylation; preparation of allylhydroxylamines by addition of alkynes to pinacolborane with subsequent dialkylzinc-promoted addition of vinylboronates to nitrones)

RN 426822-59-5 HCAPLUS

CN Methanamine, N-(2-phenylpropylidene)-, N-oxide (9CI) (CA INDEX NAME)



L28 ANSWER 5 OF 16 HCAPLUS COPYRIGHT 2005 ACS on STN

AN 2003:591307 HCAPLUS

DN 139:143997

ED Entered STN: 01 Aug 2003

TI Methods using Edg receptor modulators for the treatment of Edg receptor-associated conditions

IN Shankar, Geetha; Solow-Cordero, David; Spencer, Juliet V.; Gluchowski, Charles

PA Ceretek LLC, USA

SO PCT Int. Appl., 293 pp.

CODEN: PIXXD2

DT Patent

LA English

IC ICM C12N

CC 1-12 (Pharmacology)

Section cross-reference(s): 28

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2003062392	A2	20030731	WO 2003-US1881	20030121
	W:				
	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, UZ, VC, VN, YU, ZA, ZM, ZW				
	RW:				
	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
PRAI	US 2002-350445P	P	20020118		
	US 2002-350446P	P	20020118		
	US 2002-350447P	P	20020118		
	US 2002-350448P	P	20020118		

CLASS

PATENT NO. CLASS PATENT FAMILY CLASSIFICATION CODES

WO 2003062392 ICM C12N

OS MARPAT 139:143997

AB The invention provides a method of modulating an Edg-2, Edg-3, Ed-4 or Edg7 receptor-mediated biol. activity in a cell. A cell expressing the Edg-2, Edg-3, Edg-4 or Edg 7 receptor is contacted with a modulator of the Edg-2, Edg-3, Ed-4 or Edg 7 receptor sufficient to modulate receptor mediated biol. activity. In another aspect, the present invention provides a method for modulating an Edg-2, Edg-3, Ed-4 or Edg-7 receptor mediated biol. in a subject. A therapeutically effective amount of a modulator of the Edg-2, Edg-3, Ed-4 or Edg7 receptor is administered to the subject. Preparation of compds., e.g. 4,4,4-trifluoro-3-oxo-N-(5-phenyl-2H-pyrazol-3-yl)butyramide, is described.

ST Edg receptor modulator therapeutic; phenylpyrazolylbutyramide deriv prepn
Edg receptor modulator therapeutic

IT Animal cell line
(A431; Edg receptor modulators for treatment of Edg receptor-associated conditions)

IT Animal cell line
(CAOV-3; Edg receptor modulators for treatment of Edg receptor-associated conditions)

IT Inflammation
(Crohn's disease; Edg receptor modulators for treatment of Edg receptor-associated conditions)

IT Intestine, disease
(Crohn's; Edg receptor modulators for treatment of Edg receptor-associated conditions)

IT Receptors
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(EDG-1 (endothelial differentiation gene 1); Edg receptor modulators for treatment of Edg receptor-associated conditions)

IT Receptors
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(EDG-2 (endothelial differentiation gene 2); Edg receptor modulators for treatment of Edg receptor-associated conditions)

IT Receptors
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(EDG-3 (endothelial differentiation gene 3); Edg receptor modulators for treatment of Edg receptor-associated conditions)

IT Receptors
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(EDG-5 (endothelial differentiation gene 5); Edg receptor modulators for treatment of Edg receptor-associated conditions)

IT Receptors
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(EDG-6 (endothelial differentiation gene 6); Edg receptor modulators for treatment of Edg receptor-associated conditions)

IT Receptors
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(EDG-8 (endothelial differentiation gene 8); Edg receptor modulators for treatment of Edg receptor-associated conditions)

IT Angiogenesis
Angiogenesis inhibitors
Anti-inflammatory agents
Anti-ischemic agents
Antiasthmatics
Antimigraine agents
Antirheumatic agents
Antitumor agents
Apoptosis
Asthma
Atherosclerosis
Behcet's syndrome
Cardiovascular agents
Cardiovascular system, disease
Cell migration

Cell proliferation
 Cytotoxic agents
 Fibroblast
 Human
 Inflammation
 Ischemia
 Kidney, neoplasm
 Lung, disease
 Lung, neoplasm
 Mammary gland, neoplasm
 Neoplasm
 Ovary, neoplasm
 Pancreas, neoplasm
 Peritoneum, neoplasm
 Platelet (blood)
 Prostate gland, neoplasm
 Psoriasis
 Rheumatoid arthritis
 Stomach, neoplasm
 Thyroid gland, neoplasm
 Uterus, neoplasm
 Vasoconstriction
 Vasodilators
 Wound
 Wound healing promoters
 (Edg receptor modulators for treatment of Edg receptor-associated conditions)
 IT Carbohydrates, biological studies
 Nucleic acids
 Organic compounds, biological studies
 Peptides, biological studies
 RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
 (Edg receptor modulators for treatment of Edg receptor-associated conditions)
 IT Receptors
 RL: BSU (Biological study, unclassified); BIOL (Biological study)
 (Edg-4; Edg receptor modulators for treatment of Edg receptor-associated conditions)
 IT Receptors
 RL: BSU (Biological study, unclassified); BIOL (Biological study)
 (Edg-7; Edg receptor modulators for treatment of Edg receptor-associated conditions)
 IT Receptors
 RL: BSU (Biological study, unclassified); BIOL (Biological study)
 (Edg; Edg receptor modulators for treatment of Edg receptor-associated conditions)
 IT Animal cell line
 (HT-1080; Edg receptor modulators for treatment of Edg receptor-associated conditions)
 IT Animal cell line
 (HTC; Edg receptor modulators for treatment of Edg receptor-associated conditions)
 IT Animal cell line
 (HUVEC; Edg receptor modulators for treatment of Edg receptor-associated conditions)
 IT Chemotaxis
 (LPA-stimulated; Edg receptor modulators for treatment of Edg receptor-associated conditions)
 IT Animal cell line
 (MDA-MB-231; Edg receptor modulators for treatment of Edg receptor-associated conditions)
 IT Animal cell line
 (MDA-MB-453; Edg receptor modulators for treatment of Edg receptor-associated conditions)
 IT Animal cell line

(OV202; Edg receptor modulators for treatment of Edg receptor-associated conditions)

IT Animal cell line
(SKOV3; Edg receptor modulators for treatment of Edg receptor-associated conditions)

IT Platelet (blood)
(activation; Edg receptor modulators for treatment of Edg receptor-associated conditions)

IT Respiratory distress syndrome
(adult; Edg receptor modulators for treatment of Edg receptor-associated conditions)

IT Antiartherosclerotics
(antiatherosclerotics; Edg receptor modulators for treatment of Edg receptor-associated conditions)

IT Anemia (disease)
(autoimmune hemolytic anemia; Edg receptor modulators for treatment of Edg receptor-associated conditions)

IT Immunity
(autoimmunity; Edg receptor modulators for treatment of Edg receptor-associated conditions)

IT Lysophosphatidic acids
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(cell proliferation stimulated by; Edg receptor modulators for treatment of Edg receptor-associated conditions)

IT Carcinoma
Myoblast
Pheochromocytoma
(cell; Edg receptor modulators for treatment of Edg receptor-associated conditions)

IT Artery
(cerebral, vasoconstriction; Edg receptor modulators for treatment of Edg receptor-associated conditions)

IT Uterus, neoplasm
(cervix; Edg receptor modulators for treatment of Edg receptor-associated conditions)

IT Resolution (separation)
(chromatog.; Edg receptor modulators for treatment of Edg receptor-associated conditions)

IT Kidney, disease
(chronic glomerulonephritis; Edg receptor modulators for treatment of Edg receptor-associated conditions)

IT Temperature effects, biological
(cold, transcorneal freezing; Edg receptor modulators for treatment of Edg receptor-associated conditions)

IT Intestine, neoplasm
(colon; Edg receptor modulators for treatment of Edg receptor-associated conditions)

IT Intestine, neoplasm
(colorectal; Edg receptor modulators for treatment of Edg receptor-associated conditions)

IT Burn
(cutaneous; Edg receptor modulators for treatment of Edg receptor-associated conditions)

IT Meninges
(disease, subarachnoid hemorrhage; Edg receptor modulators for treatment of Edg receptor-associated conditions)

IT Uterus, neoplasm
(endometrium; Edg receptor modulators for treatment of Edg receptor-associated conditions)

IT Blood vessel
(endothelium; Edg receptor modulators for treatment of Edg receptor-associated conditions)

IT Epithelium
(epithelial cell; Edg receptor modulators for treatment of Edg receptor-associated conditions)

IT Carcinoma

(epithelioid; Edg receptor modulators for treatment of Edg receptor-associated conditions)

IT Sarcoma
(fibrosarcoma, cell; Edg receptor modulators for treatment of Edg receptor-associated conditions)

IT Drugs
(gastrointestinal; Edg receptor modulators for treatment of Edg receptor-associated conditions)

IT Liver, neoplasm
(hepatoma; Edg receptor modulators for treatment of Edg receptor-associated conditions)

IT Phosphatidylinositols
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(hydrolysis; Edg receptor modulators for treatment of Edg receptor-associated conditions)

IT Fatty acids, biological studies
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(level of; Edg receptor modulators for treatment of Edg receptor-associated conditions)

IT Receptors
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(lysophosphatidic acid; Edg receptor modulators for treatment of Edg receptor-associated conditions)

IT Neoplasm
(metastasis; Edg receptor modulators for treatment of Edg receptor-associated conditions)

IT Headache
(migraine; Edg receptor modulators for treatment of Edg receptor-associated conditions)

IT Nerve
(neuron; Edg receptor modulators for treatment of Edg receptor-associated conditions)

IT Kidney, disease
(non-glomerular nephrosis; Edg receptor modulators for treatment of Edg receptor-associated conditions)

IT Blood vessel, disease
(occlusion; Edg receptor modulators for treatment of Edg receptor-associated conditions)

IT Egg
(oocyte, *Xenopus laevis*; Edg receptor modulators for treatment of Edg receptor-associated conditions)

IT *Xenopus laevis*
(oocyte; Edg receptor modulators for treatment of Edg receptor-associated conditions)

IT Ovary
(ovarian cell; Edg receptor modulators for treatment of Edg receptor-associated conditions)

IT Cell activation
(platelet; Edg receptor modulators for treatment of Edg receptor-associated conditions)

IT Actins
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(polymerization; Edg receptor modulators for treatment of Edg receptor-associated conditions)

IT Intestine, neoplasm
(small; Edg receptor modulators for treatment of Edg receptor-associated conditions)

IT Blood vessel, disease
(spasm; Edg receptor modulators for treatment of Edg receptor-associated conditions)

IT Brain, disease
(stroke; Edg receptor modulators for treatment of Edg receptor-associated conditions)

IT Injury
(surface epithelial cell; Edg receptor modulators for treatment of Edg receptor-associated conditions)

IT Interleukin 8
 RL: BSU (Biological study, unclassified); BIOL (Biological study)
 (synthesis; Edg receptor modulators for treatment of Edg
 receptor-associated conditions)

IT Lupus erythematosus
 (systemic; Edg receptor modulators for treatment of Edg
 receptor-associated conditions)

IT Purpura (disease)
 (thrombocytopenic, chronic; Edg receptor modulators for treatment of
 Edg receptor-associated conditions)

IT Intestine, disease
 (ulcerative colitis; Edg receptor modulators for treatment of Edg
 receptor-associated conditions)

IT Hepatitis
 (viral, chronic active; Edg receptor modulators for treatment of Edg
 receptor-associated conditions)

IT 182762-25-0, GenBank X83864 218763-60-1, GenBank AJ000479 259476-69-2,
 GenBank AF233092 262400-57-7, GenBank AF233090 384729-36-6, GenBank
 U78192 385223-15-4, GenBank AF011466 390105-18-7, GenBank AF034780
 390174-36-4, GenBank AF233365 390523-03-2, GenBank AF317676
 392101-34-7, GenBank AF127138
 RL: BSU (Biological study, unclassified); PRP (Properties); BIOL
 (Biological study)
 (Edg receptor modulators for treatment of Edg receptor-associated
 conditions)

IT 473390-98-6
 RL: FMU (Formation, unclassified); PAC (Pharmacological activity); THU
 (Therapeutic use); BIOL (Biological study); FORM (Formation,
 nonpreparative); USES (Uses)
 (Edg receptor modulators for treatment of Edg receptor-associated
 conditions)

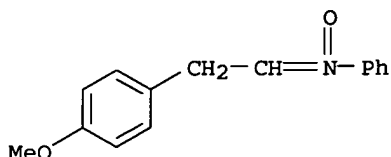
IT 353273-74-2P 569655-94-3P 569655-95-4P 569655-96-5P 569656-23-1P
 569656-24-2P
 RL: PAC (Pharmacological activity); PUR (Purification or recovery); SPN
 (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study);
 PREP (Preparation); USES (Uses)
 (Edg receptor modulators for treatment of Edg receptor-associated
 conditions)

IT 94835-69-5P
 RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic
 preparation); THU (Therapeutic use); BIOL (Biological study); PREP
 (Preparation); RACT (Reactant or reagent); USES (Uses)
 (Edg receptor modulators for treatment of Edg receptor-associated
 conditions)

IT 7741-53-9P 40622-01-3P 173275-26-8P 304650-31-5P 311799-07-2P
 312501-62-5P 312519-16-7P 331945-22-3P 334498-72-5P 342384-25-2P
 353253-35-7P 353771-45-6P 355000-90-7P 569656-08-2P 569656-09-3P
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 569656-29-7P
 RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
 (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
 (Uses)
 (Edg receptor modulators for treatment of Edg receptor-associated
 conditions)

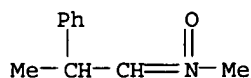
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 177360-28-0 292076-38-1 306764-68-1 309282-30-2 311773-65-6
 312594-43-7 321679-76-9 322662-05-5 327167-87-3 329350-38-1
 330630-42-7 331274-84-1 332161-39-4 337349-59-4 337469-26-8
 337498-14-3 346699-98-7 353463-50-0 353793-15-4 364051-15-0
 383164-60-1 389079-78-1 400064-03-1 569655-97-6 569655-98-7
 569656-22-0 569656-28-6
 RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL
 (Biological study); USES (Uses)
 (Edg receptor modulators for treatment of Edg receptor-associated
 conditions)

- conditions)
- IT 50-30-6, 2,6-Dichlorobenzoic acid 50-45-3, 2,3-Dichlorobenzoic acid 70-11-1, 2-Bromoacetophenone 79-19-6, Thiosemicarbazide 83-38-5, 2,6-Dichlorobenzaldehyde 91-56-5, 1H-Indole-2,3-dione 93-17-4, 3,4-Dimethoxyphenylacetonitrile 93-55-0, Propiophenone 98-59-9, p-Toluenesulfonyl chloride 98-88-4, Benzoyl chloride 98-95-3, Nitrobenzene, reactions 100-65-2, N-Phenylhydroxylamine 108-31-6, Maleic anhydride, reactions 108-38-3, 1,3-Dimethylbenzene, reactions 120-72-9, Indole, reactions 123-11-5, p-Anisaldehyde, reactions 140-75-0, 4-Fluorobenzylamine 302-01-2, Hydrazine, reactions 363-58-6 372-31-6, Ethyl 4,4,4-trifluoroacetate 406-00-8, 4-Fluorophenylhydroxylamine 434-75-3, 2-Chloro-6-fluorobenzoic acid 533-18-6, o-Tolyl acetate 556-90-1, Pseudothiohydantoin 619-05-6, 3,4-Diaminobenzoic acid 619-41-0, 2-Bromo-4'-methylacetophenone 829-20-9 1226-42-2, 4,4'-Dimethoxybenzil 1468-83-3, 3-Acetylthiophene 1476-23-9, Allyl isocyanate 1572-10-7 2642-63-9, 3',4'-Dichloroacetophenone 4506-71-2 5242-26-2 5351-85-9 6629-60-3, Ethylhydrazine oxalate 13100-05-5 13380-67-1 19541-95-8 23448-86-4 23821-37-6 36817-57-9 39151-19-4 64900-65-8, 2-Chlorobenzenesulfonyl isocyanate 72411-52-0 82799-44-8 89570-85-4 96799-03-0 96799-04-1 569656-04-8 569656-05-9 569656-06-0
- RL: RCT (Reactant); RACT (Reactant or reagent)
- (Edg receptor modulators for treatment of Edg receptor-associated conditions)
- IT 5351-91-7P 5467-70-9P 6292-74-6P 7420-34-0P 7741-54-0P 43071-45-0P 76293-13-5P 82799-45-9P 86358-85-2P 91912-53-7P 112612-58-5P 113054-02-7P 149246-80-0P 149246-86-6P 208519-10-2P 208519-15-7P 329069-72-9P 502132-61-8P 569655-99-8P 569656-00-4P 569656-01-5P 569656-02-6P 569656-03-7P **569656-07-1P**
- RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent).
- (Edg receptor modulators for treatment of Edg receptor-associated conditions)
- IT 26993-30-6, Sphingosine-1-phosphate
- RL: BSU (Biological study, unclassified); BIOL (Biological study) (calcium mobilization stimulated by; Edg receptor modulators for treatment of Edg receptor-associated conditions)
- IT 60-92-4, Cyclic AMP
- RL: BSU (Biological study, unclassified); BIOL (Biological study) (formation inhibition; Edg receptor modulators for treatment of Edg receptor-associated conditions)
- IT 7440-70-2, Calcium, biological studies
- RL: BSU (Biological study, unclassified); BIOL (Biological study) (mobilization; Edg receptor modulators for treatment of Edg receptor-associated conditions)
- IT 127464-60-2, Vascular endothelial growth factor
- RL: BSU (Biological study, unclassified); BIOL (Biological study) (synthesis; Edg receptor modulators for treatment of Edg receptor-associated conditions)
- IT **569656-07-1P**
- RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
- (Edg receptor modulators for treatment of Edg receptor-associated conditions)
- RN 569656-07-1 HCAPLUS
- CN Benzenamine, N-[2-(4-methoxyphenyl)ethylidene]-, N-oxide (9CI) (CA INDEX NAME)



L28 ANSWER 6 OF 16 HCAPLUS COPYRIGHT 2005 ACS on STN
 AN 2002:234130 HCAPLUS
 DN 136:385899
 ED Entered STN: 28 Mar 2002
 TI Dialkylzinc-Assisted Alkynylation of Nitrones
 AU Pinet, Sandra; Pandya, Shashi Urvish; Chavant, Pierre Yves; Ayling, Alexander; Vallee, Yannick
 CS LEDSS, UMR 5616, Universite J.Fourier, Grenoble, F-38041, Fr.
 SO Organic Letters (2002), 4(9), 1463-1466 ✓
 CODEN: ORLEF7; ISSN: 1523-7060
 PB American Chemical Society
 DT Journal
 LA English
 CC 25-4 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)
 OS CASREACT 136:385899
 AB Reaction of nitrones with terminal alkynes takes place readily in the presence of a substoichiometric amount of diethylzinc in toluene, affording N-propargyl-hydroxylamines in excellent yields and purity.
 ST dialkylzinc assisted alkynylation nitrone
 IT Alkynylation
 Alkynylation catalysts
 (dialkylzinc-assisted alkynylation of nitrones)
 IT Nitrones
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (dialkylzinc-assisted alkynylation of nitrones)
 IT Alkynes
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (.alpha.-; dialkylzinc-assisted alkynylation of nitrones)
 IT 557-20-0, Diethylzinc
 RL: CAT (Catalyst use); USES (Uses)
 (dialkylzinc-assisted alkynylation of nitrones)
 IT 93-53-8, 2-Phenylpropanal 103-49-1, Dibenzylamine 593-77-1,
 N-Methylhydroxylamine 627-09-8 693-02-7, 1-Hexyne 765-03-7,
 1-Dodecyne 931-49-7 1066-54-2 3376-24-7 3585-93-1 10160-87-9
 13831-03-3 14267-92-6 14918-21-9, 5-Hexynenitrile 16314-18-4
 79887-10-8
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (dialkylzinc-assisted alkynylation of nitrones)
 IT 3376-26-9P 426822-59-5P 426822-60-8P 426822-62-0P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (dialkylzinc-assisted alkynylation of nitrones)
 IT 254762-76-0P 390423-37-7P 390423-42-4P 426822-63-1P 426822-64-2P
 426822-65-3P 426822-66-4P 426822-67-5P 426822-68-6P 426822-69-7P
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 426822-75-5P 426822-76-6P 426822-77-7P 426822-78-8P 426822-79-9P
 426822-80-2P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (dialkylzinc-assisted alkynylation of nitrones)
 RE.CNT 55 THERE ARE 55 CITED REFERENCES AVAILABLE FOR THIS RECORD
 RE
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- IT 426822-59-5P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)
 (dialkylzinc-assisted alkynylation of nitrones)
- RN 426822-59-5 HCAPLUS
 CN Methanamine, N-(2-phenylpropylidene)-, N-oxide (9CI) (CA INDEX NAME)



L28 ANSWER 7 OF 16 HCAPLUS COPYRIGHT 2005 ACS on STN
 AN 2001:585631 HCAPLUS
 DN 135:318127
 ED Entered STN: 14 Aug 2001
 TI One-pot synthesis of functionalized nitrones from nitro compounds
 AU Gautheron-Chapoulaud, Valerie; Pandya, Shashi U.; Cividino, Pascale;
 Masson, Geraldine; Py, Sandrine; Vallee, Yannick
 CS LEDSS, UMR CNRS, Universite Joseph Fourier, Grenoble, 38041, Fr.
 SO Synlett (2001), (8), 1281-1283
 CODEN: SYNLES; ISSN: 0936-5214

PB Georg Thieme Verlag
 DT Journal
 LA English
 CC 21-2 (General Organic Chemistry)
 Section cross-reference(s): 34
 OS CASREACT 135:318127
 AB Zinc-mediated reduction of nitroalkanes and nitroarenes in the presence of aldehydes is an efficient method to synthesize a wide range of nitrones. This method is mild enough to accommodate a variety of functional groups. It is particularly useful when the intermediate hydroxylamines are unstable and/or watersol. We used it to prepare several aromatic, aliphatic and highly functionalized sugar-derived nitrones. Thus, nitrones $RCH:N+(O-)R_1$ [$R = Ph, 4-MeOC_6H_4, 2-(2'-BrC_6H_4CH_2O)C_6H_4$; $R_1 = Me_2CH, Me_3C, 4-MeC_6H_4, Ph$] were prepared from $RCHO$ and R_1NO_2 in 45-96% yield.
 ST glycosyl hydroxylamine prepn; hydroxylamine intermediate redn nitroalkane; redn nitroalkane zinc mediated condensation aldehyde; nitrone substituted one pot prepn
 IT Carbohydrates, preparation
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (glycosylamines, N-hydroxy; preparation of glycosyl hydroxylamines via Zn-mediated reduction of nitroalkanes/condensation with aldehydes in one-pot)
 IT Alkanes, reactions
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (nitro; preparation of nitrones from nitroalkanes via Zn-mediated reduction/condensation with aldehydes in one-pot)
 IT Condensation reaction
 Reduction
 (preparation of nitrones from nitroalkanes via Zn-mediated reduction/condensation with aldehydes in one-pot)
 IT Nitrones
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of nitrones from nitroalkanes via Zn-mediated reduction/condensation with aldehydes in one-pot)
 IT 10343-06-3, 2,3,4,6-Tetra-O-acetyl-D-glucopyranose 58645-20-8,
 2,3,4,6-Tetra-O-acetyl-D-mannopyranose 367523-78-2
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (preparation of glycosyl hydroxylamines via Zn-mediated reduction of nitroalkanes/condensation with aldehydes in one-pot)
 IT 367523-82-8P 367523-83-9P 367523-84-0P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of glycosyl hydroxylamines via Zn-mediated reduction of nitroalkanes/condensation with aldehydes in one-pot)
 IT 7440-66-6, Zinc, uses
 RL: CAT (Catalyst use); USES (Uses)
 (preparation of nitrones from nitroalkanes via Zn-mediated reduction/condensation with aldehydes in one-pot)
 IT 79-46-9, 2-Nitropropane 98-01-1, Furfural, reactions 100-52-7,
 Benzaldehyde, reactions 104-53-0, 3-Phenylpropanal 104-55-2,
 Cinnamaldehyde 123-11-5, 4-Methoxybenzaldehyde, reactions 123-38-6,
 Propanal, reactions 590-86-3, 3-Methylbutanal 594-70-7,
 2-Methyl-2-nitropropane 4221-03-8, 5-Hydroxypentanal 137266-01-4
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (preparation of nitrones from nitroalkanes via Zn-mediated reduction/condensation with aldehydes in one-pot)
 IT 3376-24-7P 10229-64-8P 66376-14-5P 93933-62-1P 109460-99-3P
 367523-76-0P 367523-77-1P 367523-79-3P 367523-80-6P
 367523-81-7P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of nitrones from nitroalkanes via Zn-mediated reduction/condensation with aldehydes in one-pot)
 IT 98-95-3, Nitrobenzene, reactions 99-99-0, 4-Methylnitrobenzene
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (preparation of nitrones from nitrobenzenes via Zn-mediated reduction/condensation with aldehydes in one-pot)
 IT 3585-93-1P 19064-77-8P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of nitrones from nitrobenzenes via Zn-mediated
reduction/condensation with aldehydes in one-pot)

RE.CNT 38 THERE ARE 38 CITED REFERENCES AVAILABLE FOR THIS RECORD
RE

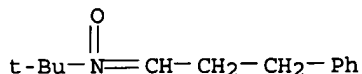
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IT 367523-81-7P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of nitrones from nitroalkanes via Zn-mediated
reduction/condensation with aldehydes in one-pot)

RN 367523-81-7 HCAPLUS

CN 2-Propanamine, 2-methyl-N-(3-phenylpropylidene)-, N-oxide (9CI) (CA INDEX
NAME)



L28 ANSWER 8 OF 16 HCAPLUS COPYRIGHT 2005 ACS on STN

AN 2000:336165 HCAPLUS

DN 133:135261

ED Entered STN: 21 May 2000

TI .alpha.,.beta.-Unsaturated Fischer carbene complexes vs. 1,3-dipoles:
reactions with nitrones and nitrilimines

AU Barluenga, Jose; Fernandez-Mari, Felix; Gonzalez, Rosario; Aguilar,

Enrique; Revelli, Gustavo A.; Viado, Argimiro L.; Fananas, Francisco J.; Olano, Bernardo

CS Instituto Universitario de Química Organometalica "Enrique Moles", Unidad Asociada al C.S.I.C., Universidad de Oviedo, Oviedo, E-33071, Spain

SO European Journal of Organic Chemistry (2000), (9), 1773-1783 ✓

CODEN: EJOCFK; ISSN: 1434-193X

PB Wiley-VCH Verlag GmbH

DT Journal

LA English

CC 28-8 (Heterocyclic Compounds (More Than One Hetero Atom))

Section cross-reference(s): 29

OS CASREACT 133:135261

AB The reaction of Me3CC.tplbond.CC(OMe):Cr(CO)5 with nitrones affords .beta.-enamino keto aldehydes by the light-promoted rearrangement of the corresponding [3+2] cycloadduct carbene complexes. On the other hand, [3+2] cycloaddn. of chiral nonracemic Fischer alkenyl carbene complexes with nitrilimines yields enantiomerically pure .DELTA.2-pyrazolines with high regio- and diastereoselectivity.

ST Fischer carbene complex addn nitrone nitrilimine; cycloaddn nitrilimine Fischer carbene complex; enamino keto aldehyde prepn; pyrazoline regioselective stereoselective prepn

IT Carbenes (methylene derivatives)
RL: RCT (Reactant); RACT (Reactant or reagent)
(chromium complexes; reaction of .alpha.,.beta.-unsatd. Fischer carbene complexes with nitrones and nitrilimines)

IT Imines
RL: RCT (Reactant); RACT (Reactant or reagent)
(cyano; reaction of .alpha.,.beta.-unsatd. Fischer carbene complexes with nitrones and nitrilimines)

IT Addition reaction
Cycloaddition reaction
(reaction of .alpha.,.beta.-unsatd. Fischer carbene complexes with nitrones and nitrilimines)

IT Nitrones
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of .alpha.,.beta.-unsatd. Fischer carbene complexes with nitrones and nitrilimines)

IT 6815-66-3 15409-32-2 93072-74-3 112763-96-9 119240-64-1
152538-60-8 166114-52-9 166114-53-0 170747-62-3 196413-56-6
210759-65-2 224630-62-0 286473-46-9 286473-47-0
286473-48-1
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of .alpha.,.beta.-unsatd. Fischer carbene complexes with nitrones and nitrilimines)

IT 210759-68-5P 210759-69-6P 210759-70-9P 210759-78-7P 210759-79-8P
286473-53-8P 286473-54-9P 286473-58-3P 286473-68-5P 286839-47-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(reaction of .alpha.,.beta.-unsatd. Fischer carbene complexes with nitrones and nitrilimines)

IT 210759-85-6P 286473-49-2P 286473-50-5P 286473-51-6P 286473-52-7P
286473-59-4P 286473-60-7P 286473-61-8P 286473-62-9P 286473-63-0P
286473-64-1P 286473-65-2P 286473-66-3P 286473-67-4P 286473-69-6P
286473-70-9P 286473-71-0P 286473-72-1P 286473-73-2P 286473-74-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(reaction of .alpha.,.beta.-unsatd. Fischer carbene complexes with nitrones and nitrilimines)

RE.CNT 78 THERE ARE 78 CITED REFERENCES AVAILABLE FOR THIS RECORD

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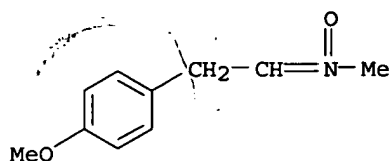
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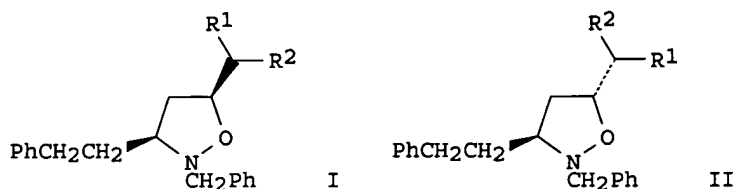
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 IT 286473-47-0
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (reaction of .alpha.,.beta.-unsatd. Fischer carbene complexes with
 nitrones and nitrilimines)
 RN 286473-47-0 HCAPLUS
 CN Methanamine, N-[2-(4-methoxyphenyl)ethylidene]-, N-oxide (9CI) (CA INDEX
 NAME)



L28 ANSWER 9 OF 16 HCAPLUS COPYRIGHT 2005 ACS on STN
 AN 1996:77508 HCAPLUS
 DN 124:232300
 ED Entered STN: 06 Feb 1996
 TI The dipolar 1,3 cycloaddition of C,N-dialkylnitron to olefins with
 hydroxyl group and the derivatives
 AU Naito, Takeaki; Shirakawa, Mitsuko; Ikai, Miho; Minomiya, Ichiya; Kiguchi,
 Toshiko
 CS Kobe Pharmaceutical Univ., Kobe, 658, Japan
 SO Recueil des Travaux Chimiques des Pays-Bas (1996), 115(1), 13-19
 CODEN: RTCPA3; ISSN: 0165-0513
 PB Elsevier
 DT Journal
 LA English
 CC 28-6 (Heterocyclic Compounds (More Than One Hetero Atom))
 Section cross-reference(s): 27
 OS CASREACT 124:232300
 GI



AB The reaction rate and stereoselectivity of intermol. dipolar 1,3
 cycloaddn. of the C,N-dialkylnitron to olefins with hydroxyl groups and
 their derivs. were found to depend upon the type of hydroxyl group. The
 rate is accelerated in the order: magnesium alkoxide (OMgBr); free
 hydroxyl group (OH); ether (OR). Selectivities are improved moderately
 when magnesium alkoxide is used. Thus, reaction of PhCH2CH2CH:N+(O-)CH2Ph
 with R1R2CHCH:CH2 [R1 = OH, OMEM, OTBDMS, NHBoc, CH2OH, CH2OTBDMS, R2 = H;
 R1 = CH2OH, R2 = NHBoc] in refluxing toluene gave adducts I and II.
 ST stereoselective dipolar cycloaddn nitron olefin; hydroxyl group effect
 dipolar cycloaddn nitron
 IT Cycloaddition reaction

Hydroxyl group

Kinetics of cycloaddition reaction

Stereochemistry

(dipolar cycloaddn. of C,N-dialkylnitron to olefins with hydroxyl group and derivs.)

IT Alkenes, reactions

Nitrones

RL: RCT (Reactant); RACT (Reactant or reagent)

(dipolar cycloaddn. of C,N-dialkylnitron to olefins with hydroxyl group and derivs.)

IT 104-53-0, Benzenepropanal 107-18-6, 2-Propen-1-ol, reactions 622-30-0,
 N-Benzylhydroxylamine 627-27-0, 3-Buten-1-ol 77120-79-7 78888-18-3,
 N-(tert-Butoxycarbonyl)allylamine 85807-85-8 108794-10-1 169324-82-7
 174714-00-2

RL: RCT (Reactant); RACT (Reactant or reagent)

(dipolar cycloaddn. of C,N-dialkylnitron to olefins with hydroxyl group and derivs.)

IT 174713-85-0P 174713-90-7P 174713-91-8P 174713-98-5P 174760-46-4P
 174760-48-6P 174760-49-7P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)

(dipolar cycloaddn. of C,N-dialkylnitron to olefins with hydroxyl group and derivs.)

IT 174713-86-1P 174713-87-2P 174713-88-3P 174713-89-4P 174713-92-9P
 174713-93-0P 174713-94-1P 174713-95-2P 174713-96-3P 174713-97-4P
 174713-99-6P 174760-47-5P 174760-50-0P 174760-51-1P

RL: SPN (Synthetic preparation); PREP (Preparation)

(dipolar cycloaddn. of C,N-dialkylnitron to olefins with hydroxyl group and derivs.)

IT 174714-00-2

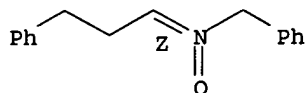
RL: RCT (Reactant); RACT (Reactant or reagent)

(dipolar cycloaddn. of C,N-dialkylnitron to olefins with hydroxyl group and derivs.)

RN 174714-00-2 HCAPLUS

CN Benzenemethanamine, N-(3-phenylpropylidene)-, N-oxide, (Z)- (9CI) (CA
 INDEX NAME)

Double bond geometry as shown.



L28 ANSWER 10 OF 16 HCAPLUS COPYRIGHT 2005 ACS on STN

AN 1994:106988 HCAPLUS

DN 120:106988

ED Entered STN: 05 Mar 1994

TI Isoxazolidine anxiolytics

IN Boyd, Edward Andrew; Costall, Brenda; Kelly, Mary Elizabeth; Parsons,
 Philip James

PA British Technology Group Ltd., UK

SO Brit. UK Pat. Appl., 45 pp.

CODEN: BAXXDU

DT Patent

LA English

IC ICM C07D261-20

ICS A61K031-42; C07D407-04

ICI C07D407-04, C07D261-20, C07D307-34

CC 28-6 (Heterocyclic Compounds (More Than One Hetero Atom))

Section cross-reference(s): 1

FAN.CNT 1

PATENT NO.

KIND

DATE

APPLICATION NO.

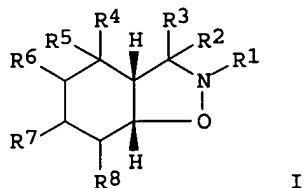
DATE

Search done by Noble Jarrell

PI	GB 2264299	A1	19930825	GB 1993-921	19930119
	GB 2264299	B2	19950726		
	IL 104771	A1	19980715	IL 1993-104771	19930217
	WO 9317004	A1	19930902	WO 1993-GB334	19930218
	W: AU, CA, JP, KR, NO, US				
	RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
	AU 9335086	A1	19930913	AU 1993-35086	19930218
	AU 677176	B2	19970417		
	EP 626951	A1	19941207	EP 1993-904218	19930218
	EP 626951	B1	19980729		
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	JP 07504181	T2	19950511	JP 1993-514623	19930218
	JP 3464479	B2	20031110		
	AT 169010	E	19980815	AT 1993-904218	19930218
	ES 2121075	T3	19981116	ES 1993-904218	19930218
	CA 2117471	C	20030422	CA 1993-2117471	19930218
	ZA 9301190	A	19940819	ZA 1993-1190	19930219
	US 5476867	A	19951219	US 1994-290752	19940815
	NO 9403042	A	19940817	NO 1994-3042	19940817
	US 5578626	A	19961126	US 1995-478142	19950607
PRAI	GB 1992-3500	A	19920219		
	GB 1993-921	A	19930119		
	WO 1993-GB334	A	19930218		
	US 1994-290752	A3	19940815		

CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
GB 2264299	ICM	C07D261-20
	ICS	A61K031-42; C07D407-04
	ICI	C07D407-04, C07D261-20, C07D307-34
GB 2264299	ECLA	C07D261/20
US 5476867	ECLA	C07D261/20; C07D413/04+307B+261
OS MARPAT 120:106988		
GI		



AB The title compds. I [R1 = H, (un)substituted C1-6 aliphatic hydrocarbyl; R2 = H; R3 = H, (un)substituted 5- or 6-membered heterocyclic aromatic ring, AR: A = straight-chain C1-4 aliphatic hydrocarbyl group; R = H, Ph, 5- or 6-membered aromatic heterocyclic ring; R4, R5 = H or together represent a C=O group; R6-R8 = H; R4 = H and 2 of R5-R8 together represent the second bond of a double bond joining position 4 and 5 or 5 and 6 or 6 and 7 with the remaining 2 of R5-R8 representing H], useful for the treatment of anxiety, the improvement of learning ability, and/or the reversal of amnesia, are prepared. Thus, N-(2-phenylethylidene)methylamine N-oxide was cyclized with 2-cyclohexenone, producing (3R,3aS,7aS)-3-benzyl-2-methyl-2,3,3a,4,5,6,7,7a-octahydrobenzo[d]isoxazol-4-one.

ST benzoisoxazolone prepn anxiolytic; amnesia treatment prepn benzoisoxazolone; isoxazolidine

IT Anxiolytics
(benzoisoxazolidines)

IT Learning
(improvement of, benzoisoxazolidines for)

IT Amnesia

(reversal of, benzoisoxazolidines for)

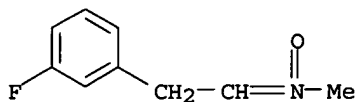
IT 152538-71-1
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (anxiolytic and amnesia reversal ability and improvement of learning ability of)

IT 152538-59-5P 152538-62-0P 152538-64-2P 152538-65-3P 152538-66-4P
 152538-68-6P 152538-69-7P 152538-70-0P 152614-34-1P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation and anxiolytic activity and amnesia reversal ability of)

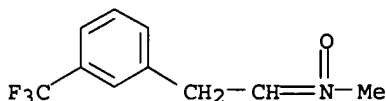
IT 110-83-8, Cyclohexene, reactions 592-57-4, 1,3-Cyclohexadiene
 930-68-7, 2-Cyclohexenone 41106-11-0, N-(Furylidene)methylamine N-oxide
 107402-94-8, N-(Ethylidene)methylamine N-oxide 152538-60-8,
 N-(2-Phenylethylidene)methylamine N-oxide 152538-61-9,
 N-(2-m-Fluorophenylethylidene)methylamine N-oxide 152538-63-1
 152538-67-5, N-(3-Phenylpropylidene)methylamine N-oxide
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (reaction of, in preparation of benzoisoxazolidines)

IT 152538-61-9, N-(2-m-Fluorophenylethylidene)methylamine N-oxide
 152538-63-1
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (reaction of, in preparation of benzoisoxazolidines)

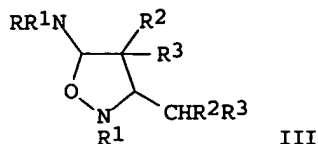
RN 152538-61-9 HCAPLUS
 CN Methanamine, N-[2-(3-fluorophenyl)ethylidene]-, N-oxide (9CI) (CA INDEX NAME)



RN 152538-63-1 HCAPLUS
 CN Methanamine, N-[2-[3-(trifluoromethyl)phenyl]ethylidene]-, N-oxide (9CI)
 (CA INDEX NAME)

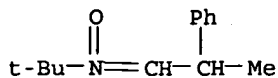


✓ L28 ANSWER 11 OF 16 HCAPLUS COPYRIGHT 2005 ACS on STN
 AN 1987:195969 HCAPLUS
 DN 106:195969
 ED Entered STN: 13 Jun 1987
 TI Aminyl oxides (Nitroxides). XXXVIII. Formation of aminyl oxides by
 oxidation of nitrones and 5-(hydroxyamino)isoxazolidines
 AU Aurich, Hans Guenter; Eidel, Joachim; Schmidt, Michael
 CS Fachbereich Chem., Univ. Marburg, Marburg, D-3550, Fed. Rep. Ger.
 SO Chemische Berichte (1986), 119(1), 36-49
 CODEN: CHBEAM; ISSN: 0009-2940
 DT Journal
 LA German
 CC 25-4 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)
 Section cross-reference(s): 28
 OS CASREACT 106:195969
 GI

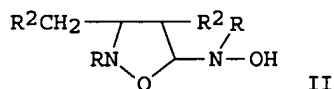


- AB According to ESR spectroscopic studies, aminyl oxides such as $R1N(O.bul.)CH:CR2R3$ (I) are formed by oxidation of nitrones $R1N(O):CHCHR2R3$ (II) or their dimers III ($R = OH$) (IV). However vinylaminyl oxides I can only be detected in the case of II ($R1 = CMe_3$, $R2 = R3 = Ph$, 3,5-(Me_3C) $2C_6H_3$; $R1 - R3 = Ph$). II ($R2 = Me$, Ph , $R3 = Me$) afford O,C-bonded spin adducts $R1N(O.bul.)CH(CHR2R3)ON(R1)CH:CR2R3$ and (or) acylaminyl oxides $R1N(O.bul.)COCHR2R3$ or $R1N(O.bul.)CHO$. Radicals III ($R = O.bul.$) (V) are formed by oxidation of IV [$R1 = Me_2C(CN)$, $R2 = H$, Me , Ph , $R3 = Me_2C(CN)$, $R2 = H$, Me , Ph , $R3 = H$; $R1 = p$ -tolyl, $R2 = Me$, $R3 = H$]. In most other cases oxidation of I or IV yields $R1N(O):CHCR2R3CH[N(R1)(O.bul.)]CHR2R3$.
- ST aminyl oxide; nitroxide; oxidn nitron; hydroxyaminoisoxazolidine oxidn; isoxazolidine hydroxyamino oxidn
- IT Oxidation
(of nitrones and hydroxyaminoisoxazolidines)
- IT Nitrones
RL: RCT (Reactant); RACT (Reactant or reagent)
(oxidation of, nitroxides from)
- IT Nitroxides
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, by oxidation of nitrones)
- IT 32798-27-9 51339-11-8 102102-03-4 108046-95-3 108046-96-4
108046-97-5 108046-98-6 108046-99-7 108047-00-3 108047-01-4
108047-02-5 108047-03-6 108047-04-7 108047-05-8 108047-06-9
108047-08-1 108047-09-2 108047-10-5 108047-11-6 108047-12-7
108047-13-8 108047-14-9 108047-15-0 108047-16-1 108047-17-2
108047-18-3
RL: PRP (Properties)
(ESR of)
- IT 52400-48-3 55830-07-4 66376-14-5 68702-72-7 72552-75-1
79566-23-7 82937-45-9 85664-55-7 85664-58-0 107323-28-4
107323-29-5 107323-32-0 107323-33-1 107323-34-2 107323-37-5
107323-41-1 107323-44-4 107323-45-5 107323-46-6 107323-48-8
107341-59-3 107341-60-6 107341-61-7 108047-25-2 108047-26-3
108069-28-9
RL: RCT (Reactant); RACT (Reactant or reagent)
(oxidation of)
- IT 82937-43-7P 108047-07-0P 108047-19-4P 108047-20-7P,
1-Benzyl-3,4-diphenyl-1H-pyrrole 108047-21-8P 108047-22-9P
108047-23-0P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation and spectra of)
- IT 14402-04-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
- IT 586-96-9 917-95-3
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with aminyloxide)
- IT 65564-72-9
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with butylidenamine oxides)
- IT 85664-58-0
RL: RCT (Reactant); RACT (Reactant or reagent)
(oxidation of)
- RN 85664-58-0 HCAPLUS
- CN 2-Propanamine, 2-methyl-N-(2-phenylpropylidene)-, N-oxide (9CI) (CA INDEX

NAME)



L28 ANSWER 12 OF 16 HCAPLUS COPYRIGHT 2005 ACS on STN
 AN 1987:176222 HCAPLUS
 DN 106:176222
 ED Entered STN: 29 May 1987
 TI The influence of steric and electronic effects on the stability of
 aldonitrone and on their conversion into isoxazolidines
 AU Aurich, Hans Guenter; Eidel, Joachim; Schmidt, Michael
 CS Fachbereich Chem., Univ. Marburg, Marburg, D-3550, Fed. Rep. Ger.
 SO Chemische Berichte (1986), 119(1), 18-35
 CODEN: CHBEAM; ISSN: 0009-2940
 DT Journal
 LA German
 CC 28-6 (Heterocyclic Compounds (More Than One Hetero Atom))
 OS CASREACT 106:176222
 GI



AB The reaction of RNHOH with R¹R²CHCHO gave R¹R²CHCH:N(O)R (I, R = Me³C, Me²CH, Me, PhCH₂; R¹ = H, R² = H, Me, Et, Ph, 3,5-(Me³C)₂C₆H₃, R¹ = R² = Me, Ph, 3,5-(Me³C)₂C₆H₃). I (R = Me³C, R² = H, Me, Et) converted slowly into isoxazolidines II, whereas all other I (R = Me³C) did not. PhNHOH reacted with R²CH₂CHO (R² = H, Me, Et, Ph) to give II. Similarly prepared were II [R = Me²C(CN), R¹ = H, R² = H, Ph]. II (R = Me³C, R² = H, Me, Et) underwent cycloreversion to give I whereas II [R = Ph, Me²C(CN)] did not. There was a steady decrease in the tendency for cycloreversion in the order II (R² = Me, R = Me³C > Me²CH > Me), however the degree of cycloreversion was also solvent dependent.

ST steric effect stability aldonitrone; electronic effect stability aldonitrone; nitronaldo stability aldonitrone; isoxazolidine hydroxyamino; hydroxylamine aldehyde condensation; cycloreversion isoxazolidine

IT Nitrones
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (aldo-, stability of, influence of steric and electronic effects on)

IT Inductive effect
 Steric effect
 (on the stability of aldonitrone)

IT 100-65-2, N-Hydroxyaniline 593-77-1 611-22-3 622-30-0,
 Benzylhydroxylamine 623-10-9 3096-63-7 5080-22-8,
 Isopropylhydroxylamine 5234-64-0 14353-69-6 16649-50-6,
 tert-Butylhydroxylamine 70853-94-0
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (condensation of, with aldehydes)

IT 75-07-0, Acetaldehyde, reactions 78-84-2, Isobutyraldehyde 93-53-8,
 2-Phenylpropionaldehyde 107-02-8, Acrolein, reactions 122-78-1,
 Phenylacetaldehyde 123-38-6, Propionaldehyde, reactions 123-72-8,
 Butyraldehyde 947-91-1 99758-86-8, 3,5-Di-tert-butylphenylacetaldehyde
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (condensation of, with hydroxylamines)

IT 62938-08-3, 3,5-Di-tert-butylbenzyl bromide

RL: RCT (Reactant); RACT (Reactant or reagent)
(coupling of)

IT 55830-07-4
RL: PRP (Properties)
(isomerization and spectra of)

IT 107323-56-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)
(preparation and acetoxylation of)

IT 107323-55-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)
(preparation and bromination of)

IT 107323-54-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and condensation of, with hydroxylamines)

IT 107323-57-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)
(preparation and hydrolysis of)

IT 107323-58-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)
(preparation and rearrangement of)

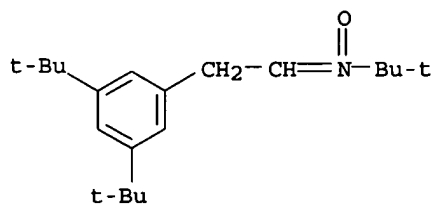
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107323-33-1P 107323-34-2P 107323-35-3P 107323-36-4P 107323-37-5P
107323-38-6P 107323-39-7P 107323-40-0P 107323-41-1P 107323-42-2P
107323-43-3P 107323-44-4P 107323-45-5P 107323-46-6P 107323-47-7P
107323-48-8P 107341-57-1P 107341-58-2P 107341-59-3P 107341-60-6P
107341-61-7P 107341-62-8P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation and spectra of)

IT 107323-53-5P 107323-60-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

IT 23259-01-0 72552-75-1 77425-84-4 79566-23-7 85664-55-7
85664-58-0 107323-49-9 107323-50-2 107323-51-3 107323-52-4
107323-59-1
RL: PRP (Properties)
(spectra of)

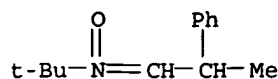
IT 107341-62-8P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation and spectra of)

RN 107341-62-8 HCAPLUS
CN 2-Propanamine, N-[2-[3,5-bis(1,1-dimethylethyl)phenyl]ethylidene]-2-methyl-, N-oxide (9CI) (CA INDEX NAME)

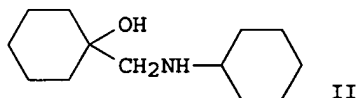


IT 85664-58-0
RL: PRP (Properties)
(spectra of)

RN 85664-58-0 HCAPLUS
CN 2-Propanamine, 2-methyl-N-(2-phenylpropylidene)-, N-oxide (9CI) (CA INDEX NAME)



L28 ANSWER 13 OF 16 HCAPLUS COPYRIGHT 2005 ACS on STN
 AN 1986:186037 HCAPLUS
 DN 104:186037
 ED Entered STN: 01 Jun 1986
 TI Preparation of vicinal N-alkylamino alcohols via acylation-rearrangement of nitrones followed by hydride reduction
 AU Coates, Robert M.; Cummins, Clark H.
 CS Dep. Chem., Univ. Illinois, Urbana, IL, 61801, USA
 SO Journal of Organic Chemistry (1986), 51(9), 1383-9
 CODEN: JOCEAH; ISSN: 0022-3263
 DT Journal
 LA English
 CC 24-7 (Alicyclic Compounds)
 Section cross-reference(s): 23
 OS CASREACT 104:186037
 GI



AB Acylation-rearrangement of N-tert-Bu and N-cyclohexyl nitrones of cyclohexanecarboxaldehyde (I), n-butyraldehyde, isobutyraldehyde, 3-cyclohexenecarboxaldehyde, and .alpha.-methylpropionaldehyde gave .alpha.-pivaloyloxy imines, which underwent reduction with LiAlH4 to N-tert-butyl- and N-cyclohexylamino alcs., e.g. II. Reduction of the .alpha.-pivaloyloxy imines derived from I with NaBH4 gave stable N-alkylamino pivalates. Acylation-rearrangement of the N-Me nitrone of I with pivaloyl chloride afforded a 3:1 mixture of the .alpha.-pivaloyloxy imine and N-pivaloyl-N-methylcyclohexanecarboxamide. It is proposed that the latter arises by elimination of an O-acyl nitrone intermediate to a nitrilium pivalate ion pair followed by collapse to an O-acyl imidate and O.fwdarw. N rearrangement. Carboxylation of the N-tert-Bu, N-cyclohexyl, and N-methylnitrones with Me chloroformate gave imino carbonates, reduction of which with sodium borohydride afforded spiro N-alkyloxazolidinones. 1-N-Methyl- and 1-(N,N-dimethylamino)methylcyclohexanol were obtained from the N-methyloxazolidinone by hydrolysis and LiAlH4 reduction, resp.

ST acylation rearrangement nitrone; alc alkylamino
 IT Rearrangement
 (acylation and, of nitrones with pivaloyl chloride)
 IT Alcohols, preparation
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (alkylamino, preparation of, via acylation-rearrangement of nitrones)
 IT Acylation
 (rearrangement and, of nitrones with pivaloyl chloride)
 IT 79-22-1
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (acylation-rearrangement by, of cyclohexanecarboxaldehyde nitrones)
 IT 3282-30-2
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (acylation-rearrangement by, of nitrones)
 IT 5857-79-4 5857-80-7 60795-42-8 72552-75-1 85664-55-7 85664-56-8
 85664-57-9 85664-58-0 89332-91-2 100812-00-8 100812-01-9

RL: RCT (Reactant); RACT (Reactant or reagent)
 (acylation-rearrangement of, with pivaloyl chloride)

IT 2719-27-9
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (amidation of, with methylamine)

IT 6830-84-8P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)
 (preparation and reaction with pivaloyl chloride)

IT 85664-60-4P 85664-61-5P 85664-62-6P 100812-02-0P 100812-03-1P
 100812-04-2P 100812-05-3P 100812-06-4P 100812-07-5P 100812-08-6P
 100812-09-7P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)
 (preparation and reduction of)

IT 100812-17-7P 100812-18-8P 100812-19-9P 100812-20-2P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)
 (preparation and reductive cyclization of)

IT 7527-65-3P 7592-90-7P 14537-89-4P 21095-16-9P 55915-75-8P
 65055-38-1P 67102-79-8P 68058-00-4P 75541-95-6P 95891-59-1P
 100812-10-0P 100812-11-1P 100812-12-2P 100812-13-3P 100812-14-4P
 100812-15-5P 100812-21-3P 100812-22-4P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)

IT 100812-16-6P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)
 (preparation, hydrolysis, and reduction of)

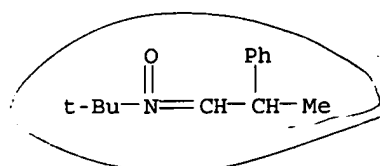
IT 4229-44-1 16649-50-6 25100-12-3
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (reaction of, with aldehydes)

IT 78-84-2 93-53-8 123-72-8 2043-61-0 42540-33-0
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (reaction of, with hydroxylamines)

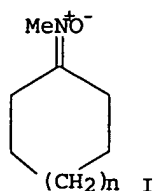
IT 85664-58-0
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (acylation-rearrangement of, with pivaloyl chloride)

RN 85664-58-0 HCAPLUS

CN 2-Propanamine, 2-methyl-N-(2-phenylpropylidene)-, N-oxide (9CI) (CA INDEX
 NAME)

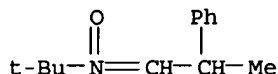


L28 ANSWER 14 OF 16 HCAPLUS COPYRIGHT 2005 ACS on STN
 AN 1983:405246 HCAPLUS
 DN 99:5246
 ED Entered STN: 12 May 1984
 TI .alpha.-Oxygenation of aldehydes and cyclic ketones by
 acylation-rearrangement of nitrones
 AU Cummins, Clark H.; Coates, Robert M.
 CS Dep. Chem., Univ. Illinois, Urbana, IL, 61801, USA
 SO Journal of Organic Chemistry (1983), 48(12), 2070-6
 CODEN: JOCEAH; ISSN: 0022-3263
 DT Journal
 LA English
 CC 24-5 (Alicyclic Compounds)
 Section cross-reference(s): 25
 OS CASREACT 99:5246
 GI



- AB Acylation of RR1CHCH:N+(O-)CMe3 (RR1CH = Pr, Me3C, cyclohexyl, 1-cyclohexen-4-yl, PhCHMe) and of nitrones I (n = 0, 1) of cyclic ketones with R2COC1 (R2 = Me, Me2CH, Me3C, Et, Ph) in the presence of NEt3 gave RR1C(O2CR2)CH:NCMe3 via rearrangement of N-vinyl-O-acylhydroxylamine intermediates. Hydrolysis of the acyloxy imines gave .alpha.-acyloxy aldehydes and ketones, e.g. EtCH(CHO)O2CR2. This acylation-rearrangement offers a new method for .alpha.-oxygenation of carbonyl compds.
- ST oxygenation aldehyde ketone; nitron acylation rearrangement; carbonyl compd oxygenation
- IT Rearrangement
(acylation and, of nitrones, oxygenated aldehydes and cyclic ketones by)
- IT Nitrones
RL: RCT (Reactant); RACT (Reactant or reagent)
(acylation-rearrangement of, oxygenated aldehydes and cyclic ketones by)
- IT Oxygenation
(of aldehydes and cyclic ketone by acylation-rearrangement of nitrones)
- IT Aldehydes, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(oxygenation of, by acylation-rearrangement of nitrones)
- IT Acylation
(rearrangement and, of nitrones, oxygenated aldehydes and cyclic ketones by)
- IT Ketones, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(cyclic, oxygenation of, by acylation-rearrangement of nitrones)
- IT 75-36-5 79-03-8 79-30-1 100-44-7, reactions 3282-30-2
RL: RCT (Reactant); RACT (Reactant or reagent)
(acylation-rearrangement by, of nitron)
- IT 72552-79-5 72552-80-8
RL: RCT (Reactant); RACT (Reactant or reagent)
(acylation-rearrangement of, oxygenated ketone by)
- IT 75-64-9, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(condensation of, with (benzoyloxy)butanal)
- IT 16649-50-6
RL: RCT (Reactant); RACT (Reactant or reagent)
(condensation of, with aldehydes and ketones)
- IT 80387-13-9
RL: RCT (Reactant); RACT (Reactant or reagent)
(condensation of, with tert-butylamine)
- IT 78-84-2 93-53-8 100-50-5 123-72-8 2043-61-0
RL: RCT (Reactant); RACT (Reactant or reagent)
(condensation of, with tert-butylhydroxylamine)
- IT 85664-63-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and acetalization of)
- IT 58751-78-3P 72552-74-0P 72552-75-1P 85664-55-7P 85664-56-8P 85664-57-9P 85664-58-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and acylation of)
 IT 82937-45-9P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (preparation and acylation-rearrangement of)
 IT 85664-59-1P 85664-60-4P 85664-61-5P 85664-75-1P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (preparation and hydrolysis of)
 IT 85664-62-6P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (preparation and hydrolysis or reduction of)
 IT 85664-65-9P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (preparation and reduction of)
 IT 85664-73-9P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (preparation and thermal rearrangement of)
 IT 15753-47-6P 55830-07-4P 65055-38-1P 85664-74-0P 85664-77-3P
 85664-78-4P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)
 IT 2522-81-8P 5921-90-4P 17472-04-7P 22094-24-2P 52789-75-0P
 55638-24-9P 56037-77-5P 60860-35-7P 85664-64-8P 85664-66-0P
 85664-67-1P 85664-68-2P 85664-69-3P 85664-70-6P 85664-71-7P
 85664-72-8P 85664-76-2P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of, via acylation-rearrangement of nitron)
 IT 85664-58-0P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (preparation and acylation of)
 RN 85664-58-0 HCAPLUS
 CN 2-Propanamine, 2-methyl-N-(2-phenylpropylidene)-, N-oxide (9CI) (CA INDEX NAME)



L28 ANSWER 15 OF 16 HCAPLUS COPYRIGHT 2005 ACS on STN

AN 1974:403566 HCAPLUS

DN 81:3566

ED Entered STN: 12 May 1984

TI Nitrones

IN Eschenmoser, Albert

PA Ciba-Geigy A.-G.

SO Ger. Offen., 24 pp.

CODEN: GWXXBX

DT Patent

LA German

IC C07C

CC 25-4 (Noncondensed Aromatic Compounds)

Section cross-reference(s): 24, 26, 27

FAN. CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	DE 2345708	A1	19740328	DE 1973-2345708	19730911
	NL 7312303	A	19740321	NL 1973-12303	19730906
	FR 2200252	A1	19740419	FR 1973-33261	19730917

	US 3894085	A	19750708	US 1973-398511	19730918
	US 3950327	A	19760413	US 1974-491197	19740724
PRAI	CH 1972-13677	A	19720919		
	CH 1972-14962	A	19721012		
	CH 1973-10652	A	19730720		
	US 1973-398511	A2	19730918		

CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
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DE 2345708	IC	C07C
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GI For diagram(s), see printed CA Issue.

AB Three RR1CHCH:N(O)R2 (I; R = Cl; R1 = H, Me; R2 = CMe3, cyclohexyl) were prepared by reaction of ClCHR1CHO with HONHR2 or by chlorination of I (R = H) with N-chlorosuccinimide. I [R = 2,5-(MeO)2C6H4, 2,5-Me2C6H4, 1-ClO7; R1 = Me; R2 = cyclohexyl] were prepared by reaction of I (R = Cl, R1 = Me, R2 = cyclohexyl) (II) with p-R2C6H4 (R = MeO, Me) and naphthalene, resp., in the presence of AgBF4 and saponified to give RR1CHCHO. Reaction of II with 4-MeC6H4OH or Ph-NHAc in the presence of AgBF4 and subsequent saponification gave by simultaneous dehydration the benzofuran III or the indole IV, resp.

ST nitron; arylpropionaldehyde; propionaldehyde aryl; benzofuran; indole; cyclohexyl nitron

IT 3376-30-5

RL: RCT (Reactant); RACT (Reactant or reagent)
(chlorination of)

IT	10410-35-2P	23543-66-0P	37898-41-2P	37898-42-3P	37898-43-4P
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52417-47-7P	52417-48-8P	52417-49-9P	52417-50-2P
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52417-51-3P	52417-52-4P	52417-53-5P	52417-54-6P
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52417-55-7P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

IT 2211-64-5 16649-50-6

RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with chloroalkanal)

IT 107-20-0 683-50-1 36884-28-3

RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with hydroxylamine derivative)

IT 103-84-4 106-44-5 150-78-7

RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with .alpha.-(chloroethyl)-N-cyclohexylnitron)

IT 91-20-3, reactions 106-42-3, reactions

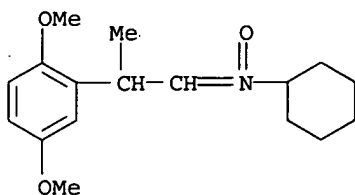
RL: RCT (Reactant); RACT (Reactant or reagent)
(with .alpha.-(chloroethyl)-N-cyclohexylnitron)

IT 52417-47-7P 52417-53-5P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

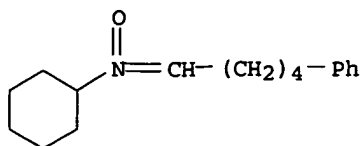
RN 52417-47-7 HCAPLUS

CN Cyclohexanamine, N-[2-(2,5-dimethoxyphenyl)propylidene]-, N-oxide (9CI)
(CA INDEX NAME)

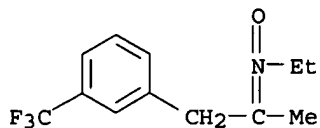


RN 52417-53-5 HCAPLUS

CN Cyclohexanamine, N-(5-phenylpentylidene)-, N-oxide (9CI) (CA INDEX NAME)



L28 ANSWER 16 OF 16 HCAPLUS COPYRIGHT 2005 ACS on STN
 AN 1974:22439 HCAPLUS
 DN 80:22439
 ED Entered STN: 12 May 1984
 TI Metabolism of amphetamines. Identification of N-oxygenated products by
 gas chromatography and mass spectrometry
 AU Beckett, A. H.; Coutts, R. T.; Ogunbona, F. A.
 CS Dep. Pharm., Chelsea Coll., London, UK
 SO Journal of Pharmacy and Pharmacology (1973), 25(9), 708-17
 CODEN: JPPMAB; ISSN: 0022-3573
 DT Journal
 LA English
 CC 1-1 (Pharmacodynamics)
 AB N-oxygenated metabolites and metabonates of amphetamines were separated and
 identified by gas chromatog.-mass spectrometry. Primary hydroxylamines
 were oxidized to oximes during gas chromatog. and could be separated and
 identified as such or could be introduced directly into the mass
 spectrometer. Secondary hydroxylamines were more stable during gas
 chromatog., although some decomposition to nitron and secondary amine did
 occur. However, oximes and nitrones did not decompose during chromatog.
 ST amphetamine metabolite mass spectra
 IT Mass spectra
 (of amphetamine oxygenated metabolites)
 IT 63-90-1 834-19-5 13213-36-0 26228-74-0 43021-97-2 43022-01-1
 43022-02-2 52271-33-7 52271-34-8 52271-35-9 52271-36-0
 52271-37-1 52271-38-2 52271-39-3 52271-40-6 52271-41-7
 52271-42-8 52271-43-9 52569-41-2
 RL: PRP (Properties)
 (mass spectrum of)
 IT 300-62-9
 RL: BIOL (Biological study)
 (oxygenated metabolites of, determination of)
 IT 52569-41-2
 RL: PRP (Properties)
 (mass spectrum of)
 RN 52569-41-2 HCAPLUS
 CN Ethanamine, N-[1-methyl-2-[3-(trifluoromethyl)phenyl]ethylidene]-, N-oxide
 (9CI) (CA INDEX NAME)



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